



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:36 pm BST

PDB ID : 1Y3A  
Title : Structure of G-Alpha-I1 bound to a GDP-selective peptide provides insight into guanine nucleotide exchange  
Authors : Johnston, C.A.; Willard, F.S.; Jezyk, M.R.; Fredericks, Z.; Bodor, E.T.; Jones, M.B.; Blaesius, R.; Harden, T.K.; Sondek, J.; Watts, V.J.; Ramer, J.K.; Siderovski, D.P.  
Deposited on : 2004-11-24  
Resolution : 2.50 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

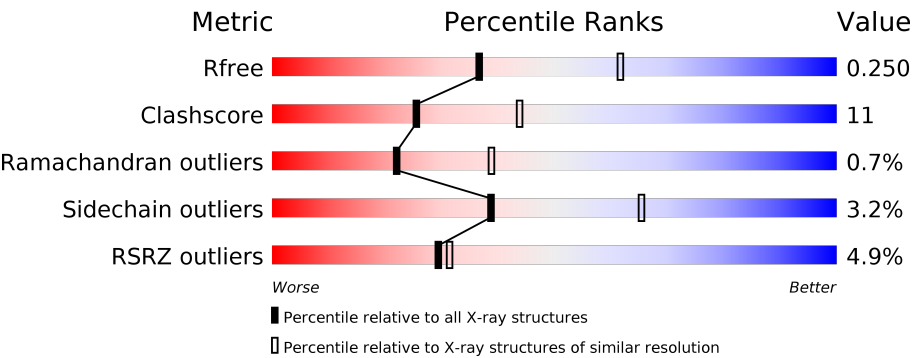
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	329	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>71%19%•9%</div></div>
1	B	329	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>73%19%•7%</div></div>
1	C	329	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>70%19%•9%</div></div>
1	D	329	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>70%20%•8%</div></div>
2	E	16	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>31%44%25%</div></div>
2	F	16	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>50%25%25%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	16	
2	H	16	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10424 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
1	A	299	Total	C	N	O	S	0	0	0
			2413	1540	407	451	15			
1	B	307	Total	C	N	O	S	0	0	0
			2471	1575	414	467	15			
1	C	298	Total	C	N	O	S	0	0	0
			2404	1534	405	450	15			
1	D	304	Total	C	N	O	S	0	0	0
			2452	1562	411	464	15			

- Molecule 2 is a protein called KB752 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	F	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	G	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			
2	H	12	Total	C	N	O	S	0	0	0
			109	71	16	21	1			

- 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	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

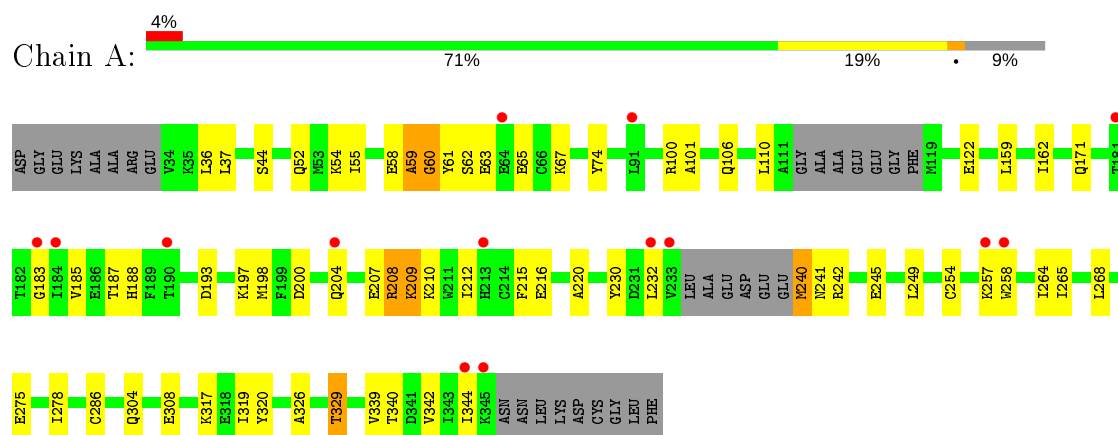
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	29	Total	O	0	0
			29	29		
4	C	30	Total	O	0	0
			30	30		
4	D	25	Total	O	0	0
			25	25		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		
4	G	2	Total	O	0	0
			2	2		
4	H	1	Total	O	0	0
			1	1		

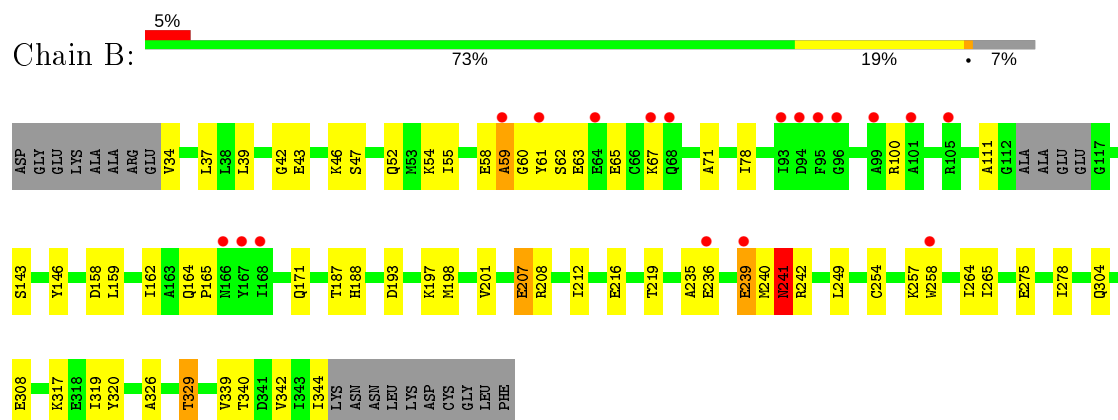
### 3 Residue-property plots [i](#)

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.

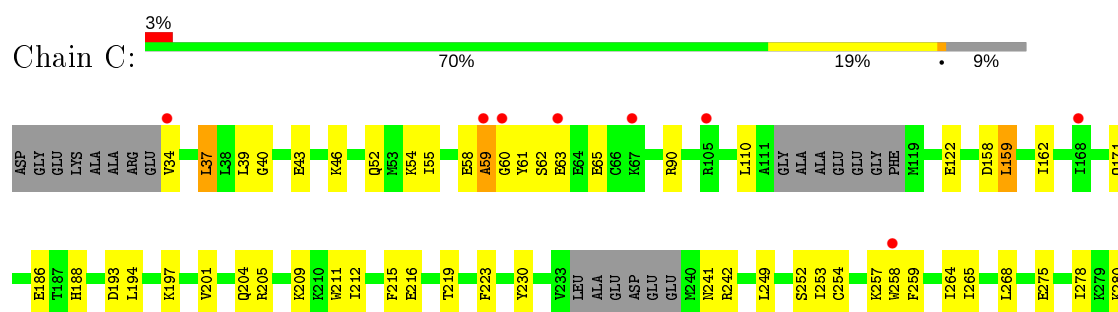
- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit



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

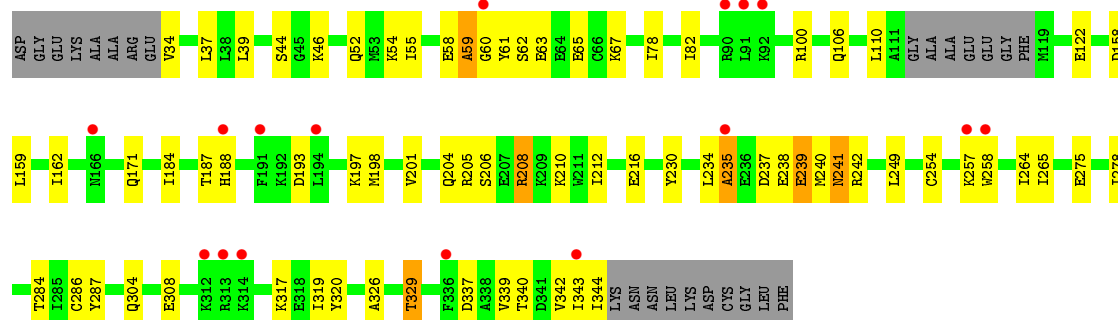


- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit





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



- Molecule 2: KB752 peptide



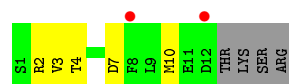
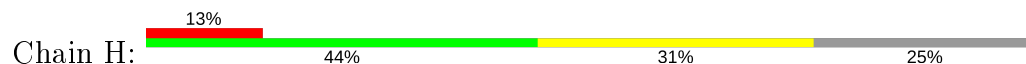
- Molecule 2: KB752 peptide



- Molecule 2: KB752 peptide



- Molecule 2: KB752 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.94Å 112.78Å 109.49Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 37.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 96.1 (37.59-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.240 , 0.280 0.244 , 0.250	Depositor DCC
$R_{free}$ test set	3001 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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

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	0.43	1/2456 (0.0%)	0.59	0/3306
1	B	0.45	1/2516 (0.0%)	0.61	0/3389
1	C	0.43	0/2447	0.60	0/3295
1	D	0.43	1/2496 (0.0%)	0.60	1/3363 (0.0%)
2	E	0.35	0/112	0.51	0/151
2	F	0.41	0/112	0.51	0/151
2	G	0.37	0/112	0.48	0/151
2	H	0.38	0/112	0.50	0/151
All	All	0.43	3/10363 (0.0%)	0.60	1/13957 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLY	N-CA	5.80	1.54	1.46
1	B	241	ASN	N-CA	5.66	1.57	1.46
1	D	241	ASN	N-CA	5.52	1.57	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	ASN	N-CA-C	-7.67	90.29	111.00

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	A	2413	0	2411	52	0
1	B	2471	0	2452	43	0
1	C	2404	0	2398	54	1
1	D	2452	0	2437	58	1
2	E	109	0	98	8	0
2	F	109	0	98	5	0
2	G	109	0	98	4	0
2	H	109	0	98	4	0
3	A	28	0	12	2	0
3	B	28	0	12	2	0
3	C	28	0	12	3	0
3	D	28	0	12	3	0
4	A	46	0	0	8	0
4	B	29	0	0	2	0
4	C	30	0	0	3	0
4	D	25	0	0	1	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	1	0
4	H	1	0	0	0	0
All	All	10424	0	10138	216	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 (216) 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:D:208:ARG:H	1:D:208:ARG:HD2	1.15	1.09
1:D:55:ILE:HA	1:D:60:GLY:HA2	1.39	1.03
1:C:55:ILE:HA	1:C:60:GLY:HA2	1.39	1.03
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.38	1.03
1:B:55:ILE:HA	1:B:60:GLY:HA2	1.38	1.02
1:A:240:MET:HG2	1:A:241:ASN:H	1.29	0.94
1:A:240:MET:HG2	1:A:241:ASN:N	1.89	0.86
1:D:339:VAL:O	1:D:342:VAL:HG12	1.74	0.85
1:C:339:VAL:O	1:C:342:VAL:HG12	1.77	0.83
1:D:235:ALA:HB3	1:D:238:GLU:HG2	1.61	0.83
1:B:339:VAL:O	1:B:342:VAL:HG12	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:HB3	4:A:360:HOH:O	1.81	0.80
1:D:264:ILE:HG12	1:D:317:LYS:HE3	1.64	0.79
1:B:264:ILE:HG12	1:B:317:LYS:HE3	1.65	0.79
1:A:339:VAL:O	1:A:342:VAL:HG12	1.81	0.79
1:D:240:MET:HG2	1:D:241:ASN:H	1.51	0.74
1:A:264:ILE:HG12	1:A:317:LYS:HE3	1.70	0.74
1:B:208:ARG:HH12	2:F:3:VAL:HG21	1.53	0.74
1:A:230:TYR:O	1:A:286:CYS:HB2	1.88	0.73
1:C:60:GLY:HA3	4:C:387:HOH:O	1.89	0.72
1:C:264:ILE:HG12	1:C:317:LYS:HE3	1.72	0.72
1:C:253:ILE:HD11	2:G:5:TRP:CZ3	2.27	0.70
1:C:90:ARG:NH2	4:C:369:HOH:O	2.22	0.70
1:D:212:ILE:O	1:D:216:GLU:HG3	1.92	0.70
2:F:3:VAL:HG13	2:F:7:ASP:HB2	1.75	0.69
1:A:232:LEU:O	4:A:357:HOH:O	2.10	0.69
1:C:110:LEU:HD11	1:C:122:GLU:HG2	1.74	0.69
2:E:3:VAL:CG1	2:E:7:ASP:HB2	2.24	0.68
1:D:240:MET:HG2	1:D:241:ASN:N	2.09	0.68
1:A:183:GLY:HA2	1:A:204:GLN:CD	2.14	0.67
1:B:39:LEU:HD23	1:B:201:VAL:HB	1.77	0.67
1:D:337:ASP:HB2	4:D:371:HOH:O	1.94	0.66
1:A:52:GLN:OE1	1:A:329:THR:HB	1.96	0.66
1:C:212:ILE:O	1:C:216:GLU:HG3	1.94	0.66
1:C:280:LYS:HG2	4:C:365:HOH:O	1.94	0.66
1:A:101:ALA:HB3	4:A:369:HOH:O	1.96	0.66
1:D:240:MET:CG	1:D:241:ASN:H	2.10	0.65
1:D:234:LEU:HD23	1:D:234:LEU:H	1.63	0.63
1:D:208:ARG:HD2	1:D:208:ARG:N	2.00	0.63
1:C:340:THR:O	1:C:344:ILE:HG12	1.99	0.63
1:C:58:GLU:O	1:C:59:ALA:CB	2.47	0.63
1:D:264:ILE:CG1	1:D:317:LYS:HE3	2.29	0.62
1:B:239:GLU:O	1:B:240:MET:HB3	1.99	0.62
1:D:58:GLU:O	1:D:59:ALA:CB	2.47	0.62
1:C:264:ILE:CG1	1:C:317:LYS:HE3	2.30	0.62
1:A:183:GLY:HA2	1:A:204:GLN:NE2	2.14	0.62
1:A:212:ILE:O	1:A:216:GLU:HG3	2.01	0.61
1:B:58:GLU:O	1:B:59:ALA:CB	2.48	0.61
1:A:58:GLU:O	1:A:59:ALA:CB	2.48	0.61
1:B:264:ILE:CG1	1:B:317:LYS:HE3	2.30	0.61
1:A:106:GLN:OE1	4:A:361:HOH:O	2.16	0.61
1:B:239:GLU:HG3	1:B:239:GLU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ARG:O	1:D:212:ILE:HG12	2.01	0.61
1:A:264:ILE:CG1	1:A:317:LYS:HE3	2.30	0.61
1:B:241:ASN:HB2	4:B:360:HOH:O	2.00	0.61
1:B:52:GLN:OE1	1:B:329:THR:HB	2.00	0.60
1:C:58:GLU:O	1:C:59:ALA:HB3	2.02	0.60
1:D:254:CYS:SG	1:D:319:ILE:HD11	2.42	0.60
1:A:265:ILE:CD1	1:A:339:VAL:HG13	2.31	0.59
1:B:58:GLU:O	1:B:59:ALA:HB3	2.03	0.59
1:C:62:SER:OG	1:C:65:GLU:HG3	2.03	0.59
1:B:326:ALA:HB3	3:B:356:GDP:N7	2.18	0.58
1:A:183:GLY:HA2	1:A:204:GLN:OE1	2.03	0.58
1:A:58:GLU:O	1:A:59:ALA:HB3	2.03	0.58
1:D:58:GLU:O	1:D:59:ALA:HB3	2.02	0.58
1:D:62:SER:OG	1:D:65:GLU:HG3	2.03	0.58
1:B:207:GLU:HA	2:F:1:SER:O	2.04	0.58
1:D:52:GLN:OE1	1:D:329:THR:HB	2.03	0.58
1:A:304:GLN:O	1:A:308:GLU:HG3	2.04	0.58
1:D:340:THR:O	1:D:344:ILE:HG12	2.03	0.58
1:B:304:GLN:O	1:B:308:GLU:HG3	2.03	0.57
1:C:205:ARG:HD2	4:G:63:HOH:O	2.04	0.57
1:C:209:LYS:HB2	1:D:237:ASP:HB3	1.87	0.57
1:B:212:ILE:O	1:B:216:GLU:HG3	2.05	0.56
1:B:254:CYS:SG	1:B:319:ILE:HD11	2.46	0.56
1:D:188:HIS:CE1	1:D:197:LYS:HD2	2.39	0.56
1:D:39:LEU:HD23	1:D:201:VAL:HB	1.87	0.56
1:A:212:ILE:HD13	2:E:8:PHE:HZ	1.70	0.56
1:A:208:ARG:O	1:A:212:ILE:HG12	2.05	0.56
1:A:254:CYS:SG	1:A:319:ILE:HD11	2.45	0.56
1:C:188:HIS:CE1	1:C:197:LYS:HD2	2.41	0.56
1:B:54:LYS:HA	1:B:58:GLU:HB2	1.87	0.56
1:A:188:HIS:CE1	1:A:197:LYS:HD2	2.40	0.56
1:C:52:GLN:OE1	1:C:329:THR:HB	2.06	0.55
1:B:62:SER:OG	1:B:65:GLU:HG3	2.06	0.55
1:C:215:PHE:CD2	1:C:259:PHE:HZ	2.24	0.55
1:D:230:TYR:O	1:D:286:CYS:HB2	2.07	0.55
1:D:240:MET:CG	1:D:241:ASN:N	2.69	0.55
2:E:3:VAL:HG12	2:E:4:THR:N	2.22	0.55
1:A:265:ILE:HD13	1:A:339:VAL:HG13	1.89	0.55
1:C:39:LEU:HD23	1:C:201:VAL:HB	1.89	0.55
2:H:3:VAL:HG12	2:H:4:THR:O	2.06	0.55
1:D:265:ILE:CD1	1:D:339:VAL:HG13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ASP:O	2:E:11:GLU:HG3	2.08	0.54
1:A:54:LYS:HA	1:A:58:GLU:HB2	1.89	0.54
1:D:205:ARG:O	2:H:2:ARG:HD2	2.07	0.53
1:C:254:CYS:SG	1:C:319:ILE:HD11	2.48	0.53
1:D:206:SER:HB3	1:D:210:LYS:HD2	1.89	0.53
1:A:62:SER:OG	1:A:65:GLU:HG3	2.09	0.53
2:F:3:VAL:HG12	2:F:4:THR:O	2.09	0.53
1:C:54:LYS:HA	1:C:58:GLU:HB2	1.91	0.53
1:B:265:ILE:HD13	1:B:339:VAL:HG13	1.91	0.52
1:C:204:GLN:H	1:C:204:GLN:CD	2.13	0.52
1:C:110:LEU:CD1	1:C:122:GLU:HG2	2.39	0.52
1:B:340:THR:O	1:B:344:ILE:HG12	2.09	0.52
2:E:3:VAL:HG11	2:E:7:ASP:HB2	1.92	0.52
1:B:39:LEU:CD2	1:B:201:VAL:HB	2.40	0.51
2:E:3:VAL:HG12	2:E:7:ASP:HB2	1.91	0.51
1:B:188:HIS:CE1	1:B:197:LYS:HD2	2.46	0.51
1:D:158:ASP:O	1:D:162:ILE:HG12	2.11	0.51
1:D:54:LYS:HA	1:D:58:GLU:HB2	1.91	0.51
1:C:326:ALA:HB3	3:C:357:GDP:N7	2.26	0.51
1:C:34:VAL:HG21	1:C:194:LEU:HD13	1.93	0.51
1:A:36:LEU:HD11	1:A:220:ALA:HB3	1.94	0.50
1:A:61:TYR:H	1:A:171:GLN:NE2	2.09	0.50
1:B:265:ILE:CD1	1:B:339:VAL:HG13	2.41	0.50
1:C:39:LEU:CD2	1:C:201:VAL:HB	2.42	0.50
1:D:265:ILE:HD13	1:D:339:VAL:HG13	1.93	0.50
1:A:257:LYS:HG3	1:A:258:TRP:CD1	2.47	0.50
1:D:257:LYS:HG3	1:D:258:TRP:CD1	2.47	0.50
1:D:304:GLN:O	1:D:308:GLU:HG3	2.12	0.50
1:A:326:ALA:HB3	3:A:355:GDP:N7	2.27	0.49
1:C:55:ILE:HA	1:C:60:GLY:CA	2.28	0.49
1:D:184:ILE:HG13	1:D:204:GLN:HE21	1.76	0.49
1:D:234:LEU:O	1:D:235:ALA:O	2.29	0.49
1:D:239:GLU:O	1:D:240:MET:HB3	2.11	0.49
1:C:320:TYR:CE1	1:C:342:VAL:HG21	2.47	0.49
1:D:326:ALA:HB3	3:D:358:GDP:N7	2.28	0.49
1:B:208:ARG:NH1	2:F:3:VAL:HG21	2.25	0.49
1:A:187:THR:HG22	1:A:198:MET:HB3	1.94	0.48
1:B:257:LYS:HG3	1:B:258:TRP:CD1	2.49	0.48
1:C:34:VAL:HG13	1:C:219:THR:HG21	1.96	0.48
1:D:110:LEU:CD1	1:D:122:GLU:HG2	2.43	0.48
1:C:304:GLN:O	1:C:308:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:344:ILE:HG12	2.14	0.48
1:A:209:LYS:HE3	1:A:209:LYS:HA	1.95	0.48
1:B:78:ILE:HG21	1:B:111:ALA:HB1	1.96	0.48
1:C:275:GLU:O	1:C:278:ILE:HG22	2.13	0.48
1:C:257:LYS:HG3	1:C:258:TRP:CD1	2.48	0.48
1:D:235:ALA:HB3	1:D:238:GLU:CG	2.39	0.47
1:D:61:TYR:H	1:D:171:GLN:NE2	2.11	0.47
1:C:40:GLY:HA2	1:C:223:PHE:CE1	2.49	0.47
1:A:36:LEU:CD1	1:A:220:ALA:HB3	2.45	0.47
1:D:44:SER:N	3:D:358:GDP:O3B	2.48	0.47
1:D:238:GLU:O	1:D:238:GLU:HG3	2.15	0.47
1:A:210:LYS:HG3	4:A:396:HOH:O	2.14	0.47
1:D:275:GLU:O	1:D:278:ILE:HG22	2.15	0.47
1:D:46:LYS:HB2	3:D:358:GDP:O1B	2.15	0.46
1:C:46:LYS:HB2	3:C:357:GDP:O1B	2.15	0.46
1:D:55:ILE:HA	1:D:60:GLY:CA	2.28	0.46
1:C:265:ILE:HD13	1:C:339:VAL:HG13	1.98	0.46
1:B:320:TYR:CE1	1:B:342:VAL:HG21	2.51	0.46
1:B:158:ASP:O	1:B:162:ILE:HG12	2.16	0.46
1:D:39:LEU:CD2	1:D:201:VAL:HB	2.46	0.46
2:H:3:VAL:HG13	2:H:7:ASP:HB2	1.97	0.46
1:A:106:GLN:HB2	4:A:361:HOH:O	2.15	0.45
1:B:34:VAL:HG13	1:B:219:THR:HG21	1.98	0.45
1:B:187:THR:HG22	1:B:198:MET:HB3	1.97	0.45
1:B:63:GLU:O	1:B:67:LYS:HG3	2.16	0.45
1:A:100:ARG:HA	1:A:100:ARG:NE	2.31	0.45
1:C:230:TYR:O	1:C:286:CYS:HB2	2.16	0.45
1:C:265:ILE:CD1	1:C:339:VAL:HG13	2.46	0.45
1:C:215:PHE:CZ	2:G:5:TRP:HB2	2.52	0.45
1:A:44:SER:N	3:A:355:GDP:O3B	2.50	0.44
1:B:275:GLU:O	1:B:278:ILE:HG22	2.18	0.44
1:C:158:ASP:O	1:C:162:ILE:HG12	2.17	0.44
1:B:239:GLU:O	1:B:240:MET:CB	2.66	0.44
1:B:55:ILE:HA	1:B:60:GLY:CA	2.27	0.44
1:A:63:GLU:O	1:A:67:LYS:HG3	2.18	0.44
1:A:110:LEU:HD13	1:A:122:GLU:HG2	1.99	0.44
1:B:100:ARG:HA	1:B:100:ARG:NE	2.33	0.44
1:C:211:TRP:O	1:C:215:PHE:HD1	2.01	0.44
1:C:212:ILE:HD13	2:G:8:PHE:HZ	1.83	0.44
1:A:215:PHE:HZ	2:E:5:TRP:HB2	1.82	0.43
1:D:63:GLU:O	1:D:67:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ILE:O	1:D:82:ILE:HG13	2.18	0.43
1:C:43:GLU:HA	3:C:357:GDP:H5"	2.00	0.43
1:D:187:THR:HG22	1:D:198:MET:HB3	2.00	0.43
1:B:71:ALA:HB3	4:B:369:HOH:O	2.18	0.43
1:A:240:MET:N	4:A:375:HOH:O	2.52	0.43
1:A:106:GLN:HG3	1:A:110:LEU:CD1	2.49	0.43
1:A:185:VAL:HB	1:A:200:ASP:HB3	2.00	0.43
1:B:61:TYR:H	1:B:171:GLN:NE2	2.16	0.43
1:D:100:ARG:NE	1:D:100:ARG:HA	2.34	0.43
1:A:320:TYR:CE1	1:A:342:VAL:HG21	2.53	0.42
1:B:46:LYS:HB2	3:B:356:GDP:O1B	2.19	0.42
1:C:61:TYR:H	1:C:171:GLN:NE2	2.16	0.42
2:H:3:VAL:HG12	2:H:4:THR:N	2.34	0.42
1:A:275:GLU:O	1:A:278:ILE:HG22	2.20	0.42
1:A:55:ILE:HA	1:A:60:GLY:CA	2.28	0.42
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.84	0.42
1:D:184:ILE:N	1:D:204:GLN:NE2	2.68	0.42
1:D:110:LEU:HD13	1:D:122:GLU:HG2	2.02	0.42
1:D:284:THR:HA	1:D:287:TYR:O	2.20	0.42
2:E:3:VAL:HG12	2:E:4:THR:H	1.83	0.42
1:C:252:SER:HB3	2:G:6:TYR:CE1	2.55	0.41
1:D:234:LEU:CD2	1:D:234:LEU:H	2.31	0.41
1:D:34:VAL:HG11	1:D:343:ILE:HD13	2.02	0.41
1:A:207:GLU:HB2	1:A:210:LYS:HE2	2.02	0.41
1:B:143:SER:HA	1:B:146:TYR:CE1	2.56	0.41
1:C:209:LYS:HD2	1:D:237:ASP:HA	2.02	0.41
1:D:106:GLN:HG3	1:D:110:LEU:HG	2.02	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.86	0.41
1:C:194:LEU:HD11	1:C:344:ILE:HD13	2.03	0.41
1:C:215:PHE:CD2	1:C:259:PHE:CZ	3.07	0.41
1:A:216:GLU:HB2	4:A:384:HOH:O	2.20	0.41
1:C:159:LEU:HD23	1:C:159:LEU:HA	1.87	0.41
1:D:320:TYR:CE1	1:D:342:VAL:HG21	2.56	0.41
1:B:42:GLY:O	1:B:43:GLU:HB2	2.21	0.41
1:C:186:GLU:OE2	1:C:188:HIS:CE1	2.73	0.41
1:C:278:ILE:HD12	1:C:278:ILE:HA	1.96	0.40
1:B:143:SER:HA	1:B:146:TYR:CZ	2.57	0.40
1:C:37:LEU:HD12	1:C:37:LEU:HA	1.90	0.40
1:A:74:TYR:HE1	1:A:162:ILE:HG22	1.86	0.40
1:B:164:GLN:HA	1:B:165:PRO:HD3	1.93	0.40
1:C:284:THR:HA	1:C:287:TYR:O	2.21	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)
1:C:63:GLU:OE1	1:D:257:LYS:NZ[2_656]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/329 (89%)	291 (99%)	1 (0%)	1 (0%)	41	61
1	B	303/329 (92%)	297 (98%)	2 (1%)	4 (1%)	12	21
1	C	292/329 (89%)	288 (99%)	2 (1%)	2 (1%)	22	39
1	D	300/329 (91%)	292 (97%)	6 (2%)	2 (1%)	22	39
2	E	10/16 (62%)	10 (100%)	0	0	100	100
2	F	10/16 (62%)	10 (100%)	0	0	100	100
2	G	10/16 (62%)	10 (100%)	0	0	100	100
2	H	10/16 (62%)	9 (90%)	1 (10%)	0	100	100
All	All	1228/1380 (89%)	1207 (98%)	12 (1%)	9 (1%)	22	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	C	241	ASN
1	D	235	ALA
1	A	59	ALA
1	B	59	ALA
1	C	59	ALA
1	D	59	ALA
1	B	236	GLU
1	B	235	ALA



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/284 (93%)	254 (97%)	9 (3%)	37	63
1	B	268/284 (94%)	258 (96%)	10 (4%)	34	60
1	C	262/284 (92%)	256 (98%)	6 (2%)	50	76
1	D	267/284 (94%)	259 (97%)	8 (3%)	41	68
2	E	12/16 (75%)	11 (92%)	1 (8%)	11	22
2	F	12/16 (75%)	12 (100%)	0	100	100
2	G	12/16 (75%)	12 (100%)	0	100	100
2	H	12/16 (75%)	11 (92%)	1 (8%)	11	22
All	All	1108/1200 (92%)	1073 (97%)	35 (3%)	39	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	159	LEU
1	A	193	ASP
1	A	208	ARG
1	A	209	LYS
1	A	240	MET
1	A	242	ARG
1	A	249	LEU
1	A	329	THR
1	B	37	LEU
1	B	47	SER
1	B	159	LEU
1	B	193	ASP
1	B	207	GLU
1	B	239	GLU
1	B	241	ASN
1	B	242	ARG
1	B	249	LEU
1	B	329	THR

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Mol	Chain	Res	Type
1	C	37	LEU
1	C	159	LEU
1	C	193	ASP
1	C	242	ARG
1	C	249	LEU
1	C	329	THR
1	D	37	LEU
1	D	159	LEU
1	D	193	ASP
1	D	208	ARG
1	D	239	GLU
1	D	242	ARG
1	D	249	LEU
1	D	329	THR
2	E	10	MET
2	H	10	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	106	GLN
1	A	147	GLN
1	A	171	GLN
1	A	241	ASN
1	A	333	GLN
1	B	79	GLN
1	B	147	GLN
1	B	171	GLN
1	B	241	ASN
1	B	333	GLN
1	C	79	GLN
1	C	147	GLN
1	C	171	GLN
1	C	204	GLN
1	C	241	ASN
1	C	333	GLN
1	D	79	GLN
1	D	147	GLN
1	D	171	GLN
1	D	213	HIS
1	D	241	ASN

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Mol	Chain	Res	Type
1	D	333	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](#)

4 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	A	355	-	24,30,30	1.86	6 (25%)	31,47,47	3.03	15 (48%)
3	GDP	B	356	-	24,30,30	1.94	7 (29%)	31,47,47	3.03	15 (48%)
3	GDP	C	357	-	24,30,30	1.75	5 (20%)	31,47,47	3.03	14 (45%)
3	GDP	D	358	-	24,30,30	1.79	6 (25%)	31,47,47	3.06	15 (48%)

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	A	355	-	-	3/12/32/32	0/3/3/3
3	GDP	B	356	-	-	3/12/32/32	0/3/3/3
3	GDP	C	357	-	-	3/12/32/32	0/3/3/3
3	GDP	D	358	-	-	3/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	356	GDP	C6-N1	6.20	1.43	1.33
3	D	358	GDP	C6-N1	5.63	1.42	1.33
3	C	357	GDP	C6-N1	5.47	1.42	1.33
3	A	355	GDP	C6-N1	5.42	1.42	1.33
3	A	355	GDP	O4'-C1'	2.82	1.45	1.41
3	D	358	GDP	C5'-C4'	2.77	1.60	1.51
3	A	355	GDP	C2-N1	2.70	1.40	1.35
3	D	358	GDP	C8-N7	-2.65	1.30	1.34
3	A	355	GDP	C8-N7	-2.65	1.30	1.34
3	B	356	GDP	C5'-C4'	2.62	1.59	1.51
3	A	355	GDP	C5'-C4'	2.61	1.59	1.51
3	B	356	GDP	C8-N7	-2.57	1.30	1.34
3	B	356	GDP	C2-N1	2.49	1.39	1.35
3	B	356	GDP	O4'-C1'	2.48	1.44	1.41
3	A	355	GDP	C3'-C4'	2.48	1.59	1.53
3	C	357	GDP	C8-N7	-2.44	1.30	1.34
3	C	357	GDP	C5'-C4'	2.42	1.59	1.51
3	B	356	GDP	C3'-C4'	2.41	1.59	1.53
3	C	357	GDP	C3'-C4'	2.37	1.59	1.53
3	C	357	GDP	C2-N1	2.28	1.39	1.35
3	D	358	GDP	C3'-C4'	2.26	1.58	1.53
3	D	358	GDP	O4'-C1'	2.15	1.44	1.41
3	B	356	GDP	PA-O2A	-2.03	1.45	1.55
3	D	358	GDP	C2-N1	2.03	1.39	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	355	GDP	C5-C6-N1	-8.48	111.84	123.43
3	D	358	GDP	C5-C6-N1	-8.28	112.10	123.43
3	B	356	GDP	C5-C6-N1	-8.22	112.19	123.43
3	C	357	GDP	C5-C6-N1	-8.05	112.42	123.43
3	C	357	GDP	O5'-PA-O1A	-7.57	79.48	109.07
3	B	356	GDP	O5'-PA-O1A	-7.50	79.75	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	358	GDP	O5'-PA-O1A	-7.49	79.80	109.07
3	A	355	GDP	O5'-PA-O1A	-7.44	80.01	109.07
3	D	358	GDP	C6-N1-C2	5.94	125.37	115.93
3	B	356	GDP	C6-N1-C2	5.86	125.24	115.93
3	A	355	GDP	C6-N1-C2	5.74	125.06	115.93
3	C	357	GDP	C6-N1-C2	5.67	124.94	115.93
3	C	357	GDP	O3B-PB-O3A	4.65	120.24	104.64
3	D	358	GDP	O3B-PB-O3A	4.44	119.54	104.64
3	A	355	GDP	O3B-PB-O3A	4.43	119.48	104.64
3	B	356	GDP	O3B-PB-O3A	4.34	119.18	104.64
3	B	356	GDP	C2-N3-C4	-3.77	111.06	115.36
3	C	357	GDP	O2A-PA-O1A	3.65	130.28	112.24
3	D	358	GDP	C2-N3-C4	-3.60	111.24	115.36
3	B	356	GDP	O2A-PA-O1A	3.56	129.82	112.24
3	D	358	GDP	O2A-PA-O1A	3.55	129.79	112.24
3	A	355	GDP	C2-N3-C4	-3.50	111.36	115.36
3	C	357	GDP	C2-N3-C4	-3.45	111.41	115.36
3	A	355	GDP	O2A-PA-O1A	3.42	129.14	112.24
3	B	356	GDP	O4'-C4'-C3'	-3.14	98.89	105.11
3	A	355	GDP	O4'-C4'-C3'	-3.12	98.94	105.11
3	C	357	GDP	O4'-C4'-C3'	-3.08	99.01	105.11
3	D	358	GDP	C6-C5-C4	-3.08	117.86	120.80
3	C	357	GDP	N3-C2-N1	-3.03	123.18	127.22
3	D	358	GDP	O4'-C4'-C3'	-3.03	99.12	105.11
3	D	358	GDP	N3-C2-N1	-3.01	123.21	127.22
3	B	356	GDP	N3-C2-N1	-2.99	123.24	127.22
3	B	356	GDP	C6-C5-C4	-2.98	117.96	120.80
3	C	357	GDP	C6-C5-C4	-2.97	117.96	120.80
3	A	355	GDP	PA-O5'-C5'	2.96	139.05	121.68
3	A	355	GDP	C6-C5-C4	-2.93	118.00	120.80
3	B	356	GDP	PA-O5'-C5'	2.86	138.46	121.68
3	A	355	GDP	PA-O3A-PB	-2.82	123.15	132.83
3	D	358	GDP	PA-O5'-C5'	2.81	138.15	121.68
3	A	355	GDP	N3-C2-N1	-2.77	123.53	127.22
3	C	357	GDP	PA-O5'-C5'	2.67	137.31	121.68
3	C	357	GDP	PA-O3A-PB	-2.65	123.74	132.83
3	C	357	GDP	C1'-N9-C4	-2.60	122.08	126.64
3	C	357	GDP	O2A-PA-O5'	-2.59	95.72	107.75
3	D	358	GDP	O2A-PA-O5'	-2.57	95.83	107.75
3	D	358	GDP	PA-O3A-PB	-2.49	124.27	132.83
3	B	356	GDP	PA-O3A-PB	-2.49	124.27	132.83
3	D	358	GDP	C1'-N9-C4	-2.44	122.36	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	356	GDP	O2A-PA-O5'	-2.41	96.55	107.75
3	B	356	GDP	C1'-N9-C4	-2.36	122.50	126.64
3	A	355	GDP	O5'-C5'-C4'	-2.20	101.41	108.99
3	B	356	GDP	O5'-C5'-C4'	-2.19	101.47	108.99
3	A	355	GDP	O3B-PB-O2B	-2.17	99.33	107.64
3	C	357	GDP	O5'-C5'-C4'	-2.14	101.64	108.99
3	A	355	GDP	C1'-N9-C4	-2.11	122.93	126.64
3	D	358	GDP	O3B-PB-O2B	-2.10	99.60	107.64
3	D	358	GDP	O5'-C5'-C4'	-2.07	101.87	108.99
3	A	355	GDP	O2A-PA-O5'	-2.02	98.34	107.75
3	B	356	GDP	O3B-PB-O2B	-2.01	99.96	107.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	355	GDP	O4'-C4'-C5'-O5'
3	B	356	GDP	O4'-C4'-C5'-O5'
3	C	357	GDP	O4'-C4'-C5'-O5'
3	D	358	GDP	O4'-C4'-C5'-O5'
3	A	355	GDP	C3'-C4'-C5'-O5'
3	B	356	GDP	C3'-C4'-C5'-O5'
3	D	358	GDP	C3'-C4'-C5'-O5'
3	C	357	GDP	C3'-C4'-C5'-O5'
3	A	355	GDP	PB-O3A-PA-O2A
3	B	356	GDP	PB-O3A-PA-O2A
3	C	357	GDP	PB-O3A-PA-O2A
3	D	358	GDP	PB-O3A-PA-O2A

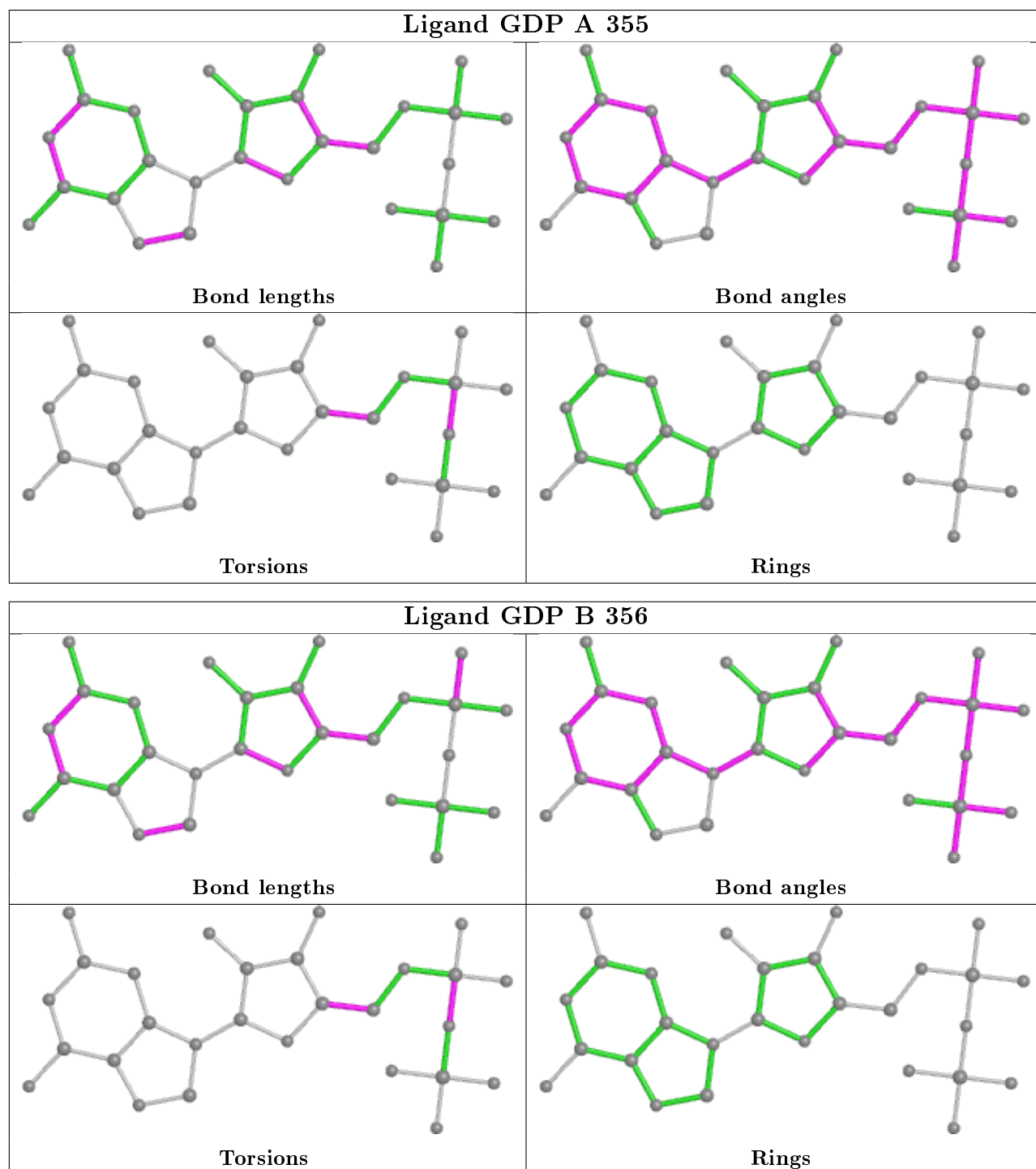
There are no ring outliers.

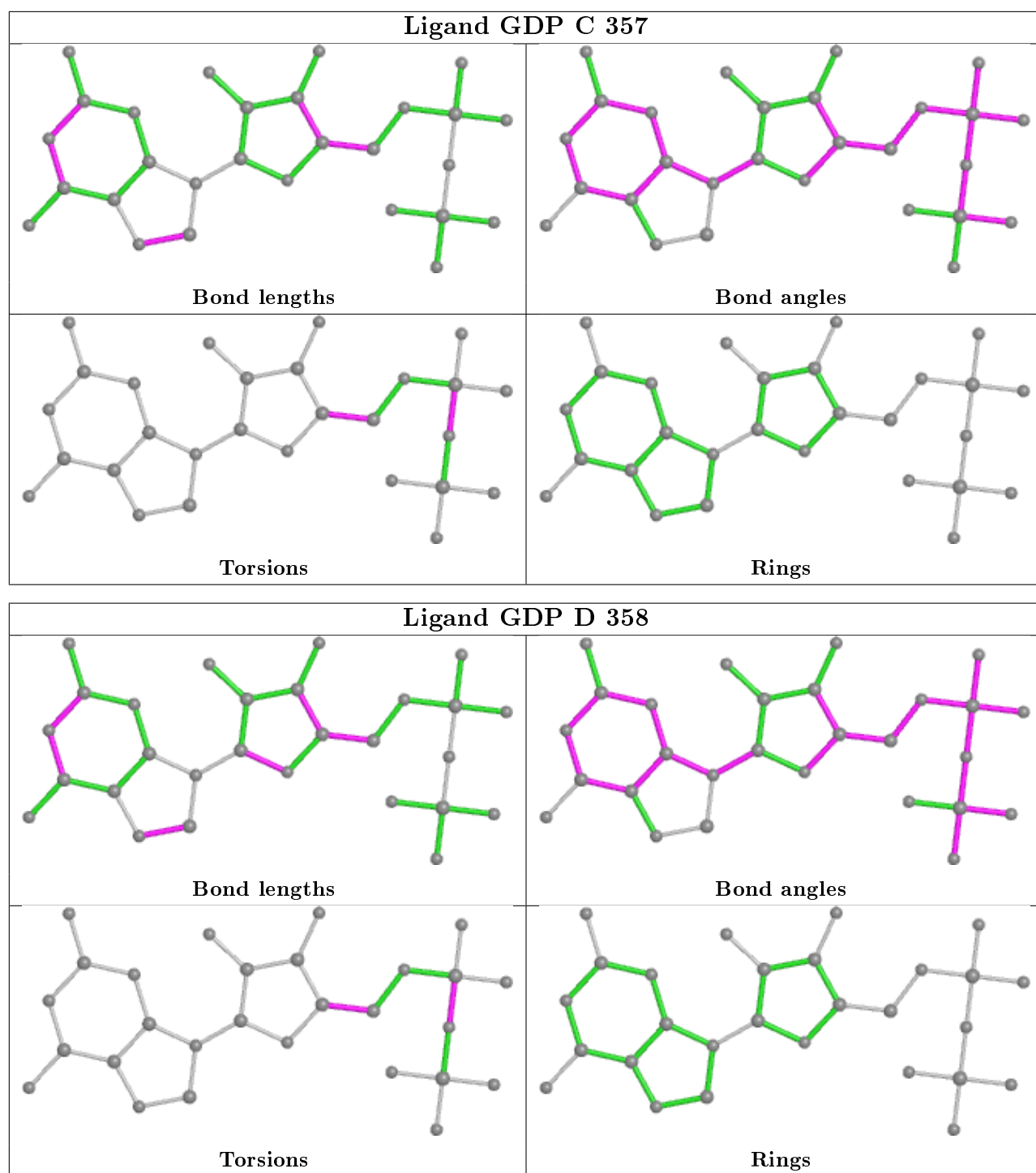
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	355	GDP	2	0
3	B	356	GDP	2	0
3	C	357	GDP	3	0
3	D	358	GDP	3	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	299/329 (90%)	0.28	14 (4%) 31 33	19, 40, 85, 154	0
1	B	307/329 (93%)	0.18	18 (5%) 22 23	16, 37, 78, 136	0
1	C	298/329 (90%)	0.15	10 (3%) 45 48	21, 38, 80, 104	0
1	D	304/329 (92%)	0.31	16 (5%) 26 28	22, 43, 96, 171	0
2	E	12/16 (75%)	1.20	2 (16%) 1 1	43, 64, 84, 142	0
2	F	12/16 (75%)	-0.04	0 100 100	24, 44, 69, 110	0
2	G	12/16 (75%)	0.22	0 100 100	34, 48, 91, 130	0
2	H	12/16 (75%)	0.99	2 (16%) 1 1	43, 66, 100, 148	0
All	All	1256/1380 (91%)	0.25	62 (4%) 29 31	16, 40, 85, 171	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	257	LYS	6.2
1	D	258	TRP	5.5
1	C	59	ALA	4.8
1	A	345	LYS	4.7
2	E	12	ASP	4.5
1	C	67	LYS	4.3
1	C	258	TRP	4.2
2	H	8	PHE	3.8
1	A	258	TRP	3.7
1	A	233	VAL	3.7
1	D	194	LEU	3.4
1	B	168	ILE	3.4
1	A	344	ILE	3.4
1	D	60	GLY	3.3
1	C	60	GLY	3.3
1	B	64	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	LYS	3.2
1	C	168	ILE	3.1
1	B	95	PHE	3.1
1	C	105	ARG	3.0
1	B	94	ASP	3.0
1	D	312	LYS	3.0
1	B	167	TYR	2.9
1	B	96	GLY	2.9
1	A	181	THR	2.9
1	D	92	LYS	2.9
1	B	236	GLU	2.9
1	C	34	VAL	2.8
1	A	91	LEU	2.8
1	D	188	HIS	2.8
1	A	204	GLN	2.7
1	B	166	ASN	2.7
1	D	314	LYS	2.7
1	D	166	ASN	2.7
1	C	63	GLU	2.6
1	A	190	THR	2.6
1	D	191	PHE	2.6
1	A	232	LEU	2.6
1	B	105	ARG	2.5
1	B	101	ALA	2.5
1	D	91	LEU	2.4
1	B	61	TYR	2.4
1	C	344	ILE	2.4
1	B	99	ALA	2.3
1	B	258	TRP	2.3
1	D	343	ILE	2.3
1	D	235	ALA	2.3
1	B	68	GLN	2.2
1	B	93	ILE	2.2
1	A	183	GLY	2.2
1	C	342	VAL	2.2
1	B	239	GLU	2.2
1	B	67	LYS	2.2
1	A	64	GLU	2.2
2	H	12	ASP	2.1
1	A	213	HIS	2.1
1	D	90	ARG	2.1
1	A	184	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	336	PHE	2.1
1	D	313	ARG	2.1
2	E	8	PHE	2.0
1	B	59	ALA	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](#)

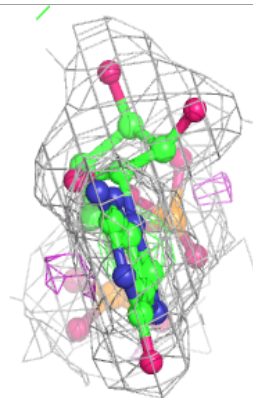
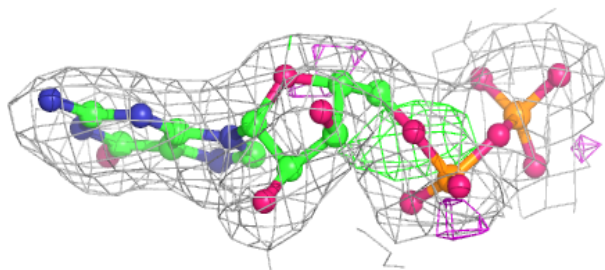
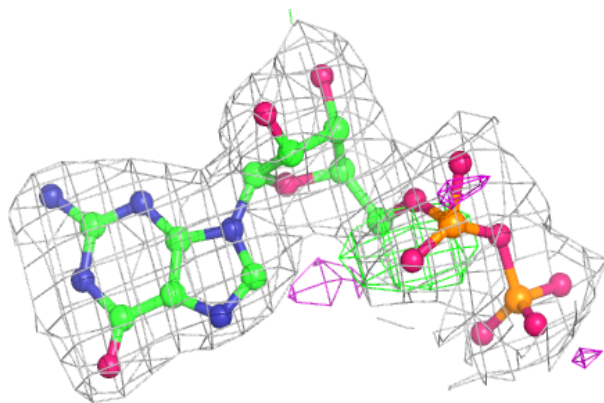
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	C	357	28/28	0.93	0.18	25,31,58,58	0
3	GDP	B	356	28/28	0.94	0.18	23,30,48,51	0
3	GDP	A	355	28/28	0.94	0.18	23,31,49,50	0
3	GDP	D	358	28/28	0.95	0.17	28,35,56,59	0

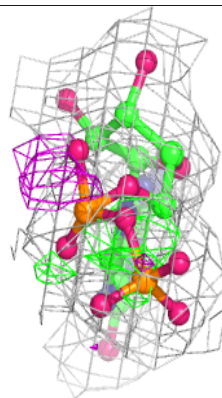
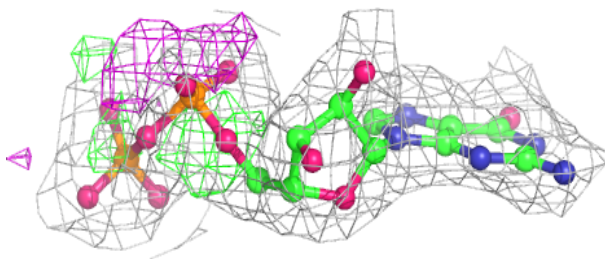
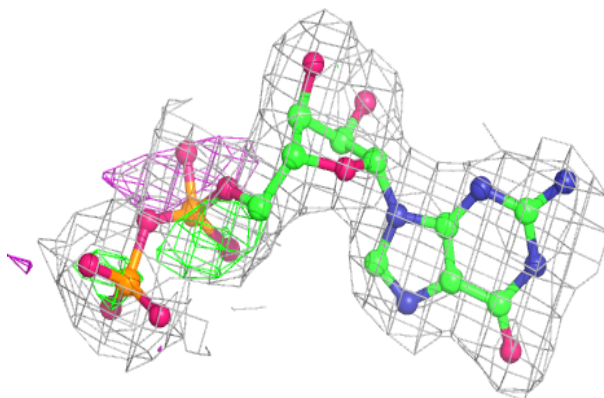
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP C 357:**

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

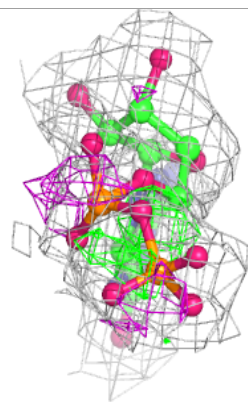
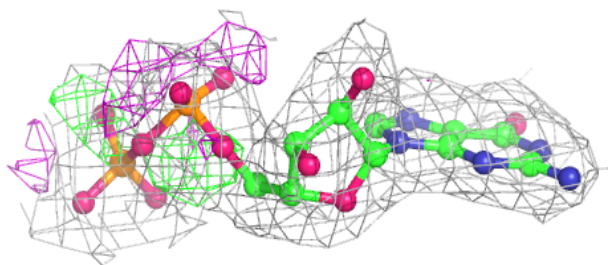
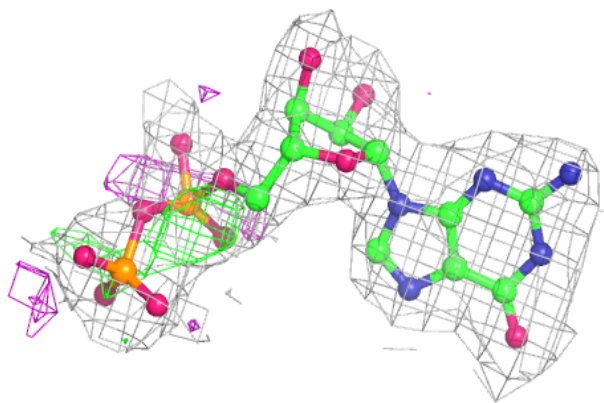
**Electron density around GDP B 356:**

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

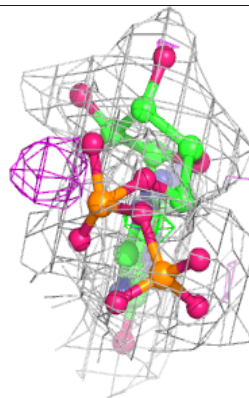
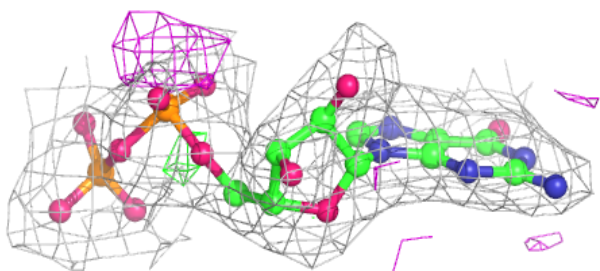
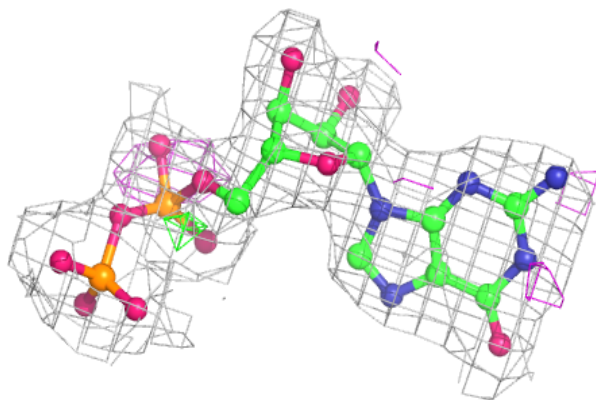


**Electron density around GDP A 355:**

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

**Electron density around GDP D 358:**

$2mF_o-DF_c$  (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.