



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 06:11 AM EDT

PDB ID : 5CJV  
Title : Isobutyryl-CoA mutase fused with bound adenosylcobalamin, GDP, Mg (holo-IcmF/GDP), and substrate isovaleryl-coenzyme A  
Authors : Jost, M.; Drennan, C.L.  
Deposited on : 2015-07-15  
Resolution : 3.45 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

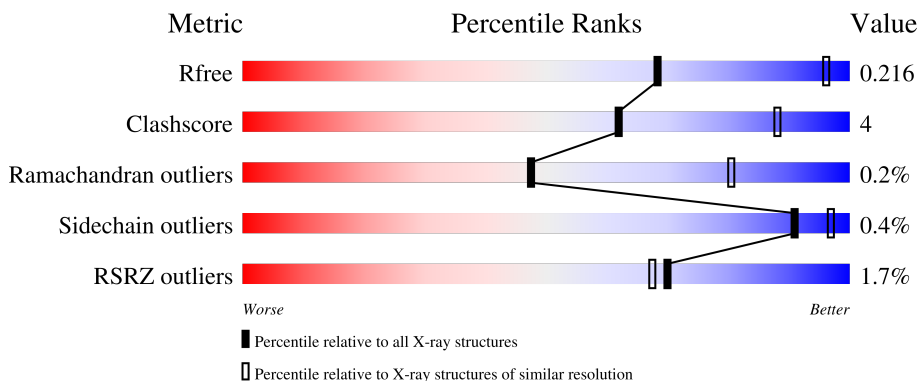
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


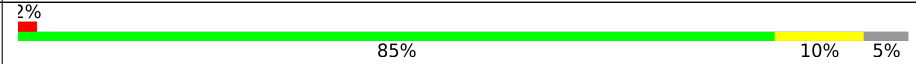
The reported resolution of this entry is 3.45 Å.

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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	1113	 84% 11% 5%
1	B	1113	 85% 10% 5%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 16519 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 Isobutyryl-CoA mutase fused.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1061	8093	5058	1449	1549	37	0	0	0
1	B	1059	8067	5034	1453	1543	37	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

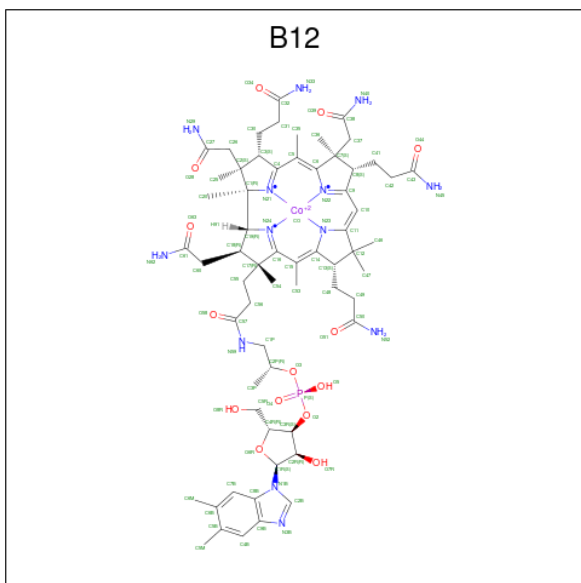
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0
B	-17	SER	-	expression tag	UNP Q1LRY0
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0

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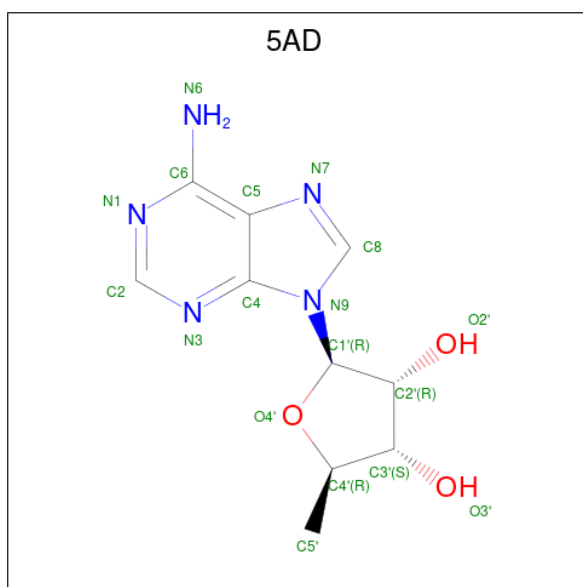
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



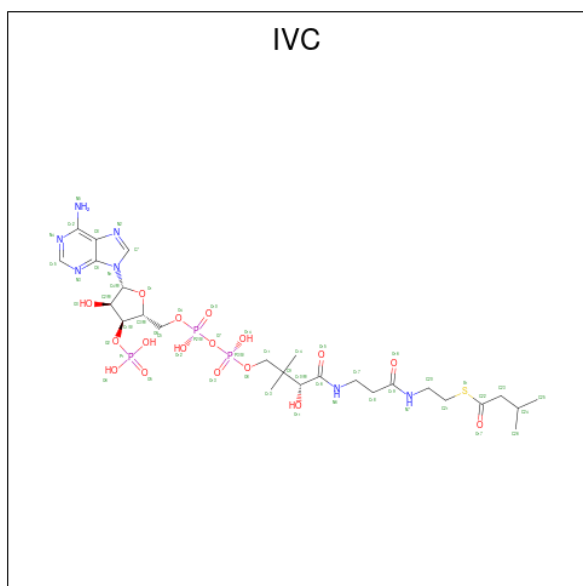
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	36	20	10	6	0	1

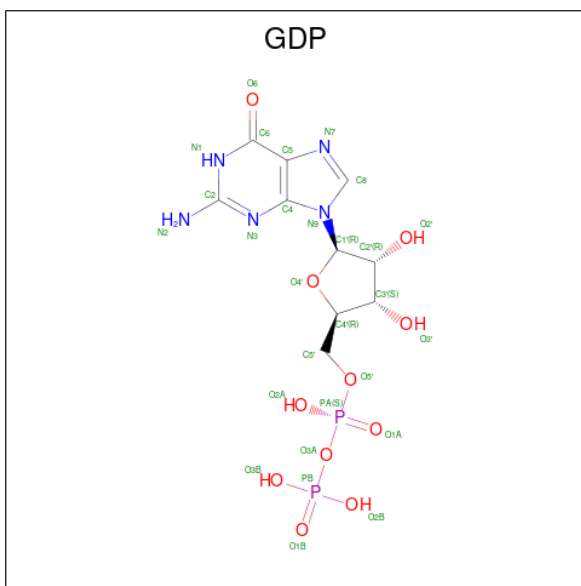
- Molecule 4 is Isovaleryl-coenzyme A (three-letter code: IVC) (formula:  $C_{26}H_{44}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	54	26	7	17	3	1	0	0
4	B	1	27	10	5	10	2		0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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		
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

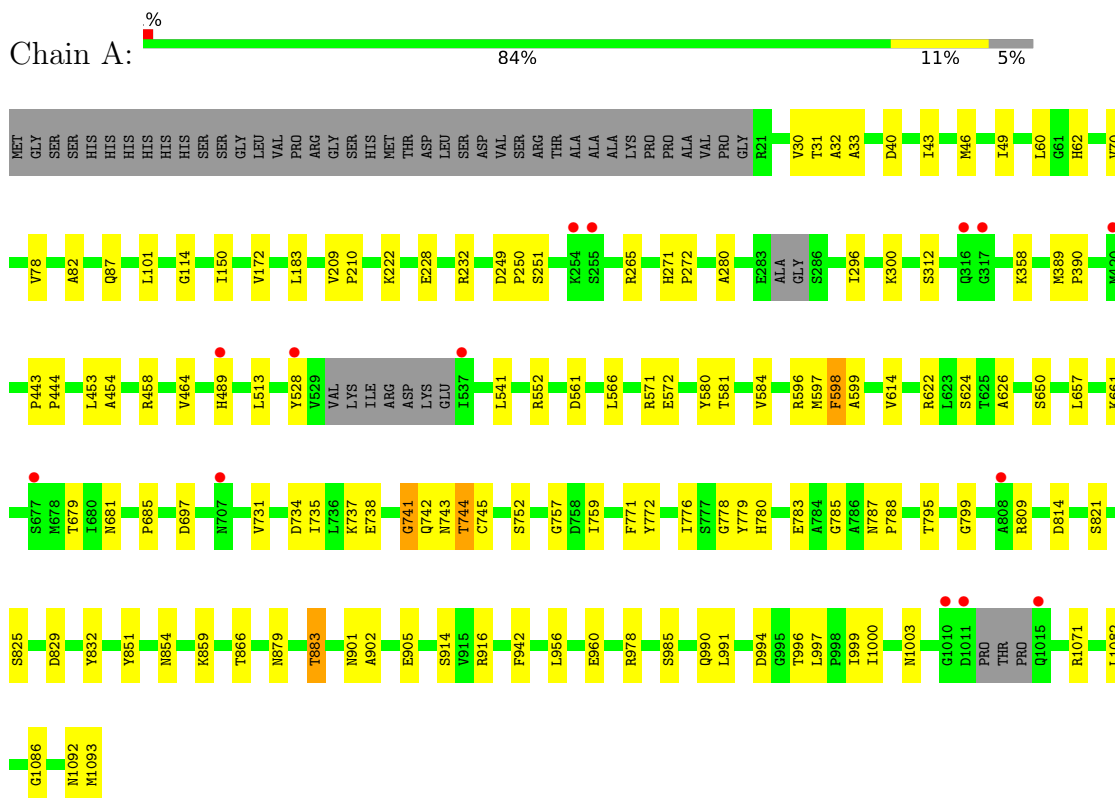
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	Total	Mg	0	0
			2	2		
6	B	2	Total	Mg	0	0
			2	2		

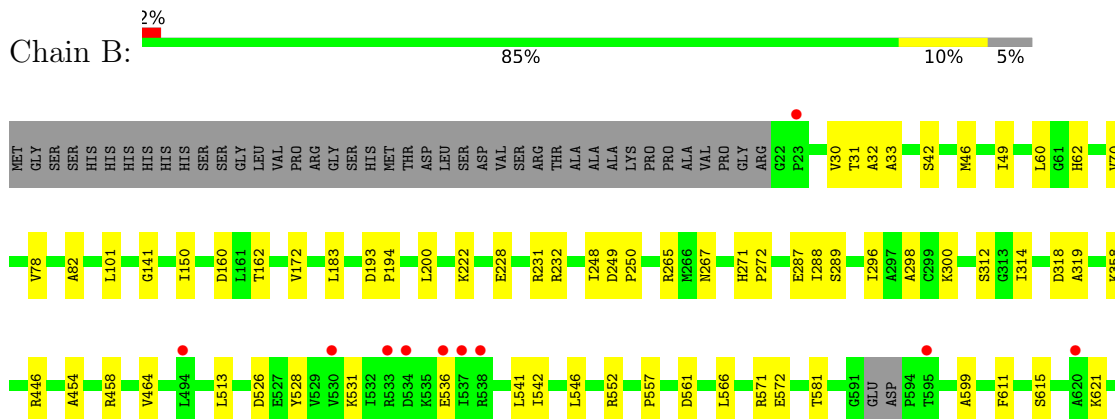
### 3 Residue-property plots [i](#)

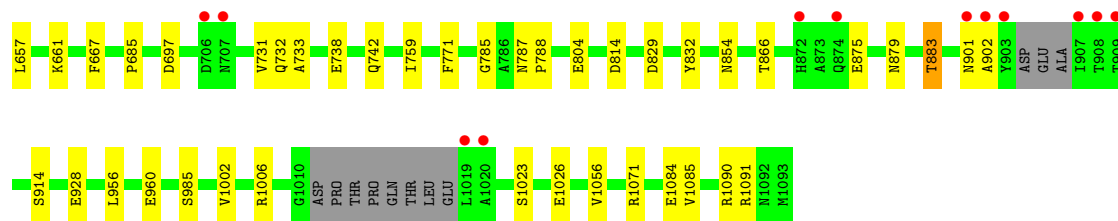
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Isobutyryl-CoA mutase fused



- Molecule 1: Isobutyryl-CoA mutase fused







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	317.56Å 317.56Å 343.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.91 – 3.45 34.91 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.91-3.45) 99.1 (34.91-3.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.47Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.193 , 0.214 0.195 , 0.216	Depositor DCC
$R_{free}$ test set	4357 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.2	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, MG, IVC, 5AD, B12

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	0.21	0/8234	0.40	3/11154 (0.0%)
1	B	0.21	0/8205	0.39	3/11107 (0.0%)
All	All	0.21	0/16439	0.39	6/22261 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	552	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	552	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	B	552	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	B	552	ARG	CD-NE-CZ	5.34	131.07	123.60
1	A	552	ARG	CD-NE-CZ	5.21	130.89	123.60

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	8093	0	7834	81	0
1	B	8067	0	7806	59	0
2	A	91	0	88	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	91	0	88	6	0
3	A	36	0	26	3	0
4	A	54	0	42	7	0
4	B	27	0	13	0	0
5	A	28	0	12	3	0
5	B	28	0	12	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	16519	0	15921	144	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 4.

All (144) 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:87:GLN:HE22	2:A:1101:B12:H421	1.44	0.82
1:A:783:GLU:HB3	2:A:1101:B12:H532	1.64	0.78
1:B:615:SER:O	1:B:621:LYS:NZ	2.25	0.69
1:A:779:TYR:OH	3:A:1102[B]:5AD:O3'	2.13	0.66
1:A:821:SER:HG	4:A:1103:IVC:H25	1.39	0.66
1:A:734:ASP:HB3	1:A:737:LYS:HZ2	1.65	0.62
1:B:314:ILE:HG23	1:B:318:ASP:HB2	1.81	0.62
1:A:681:ASN:ND2	1:A:742:GLN:OE1	2.32	0.62
1:A:31:THR:HG22	1:A:82:ALA:HB3	1.82	0.61
1:A:622:ARG:NH1	4:A:1103:IVC:O13	2.24	0.60
1:A:991:LEU:HD22	1:A:996:THR:HB	1.84	0.59
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.83	0.59
1:B:454:ALA:HA	1:B:956:LEU:HD22	1.84	0.59
1:A:735:ILE:HG13	1:A:752:SER:HB3	1.85	0.58
1:A:990:GLN:O	1:A:994:ASP:HB2	2.02	0.58
1:A:780:HIS:HA	2:A:1101:B12:H461	1.86	0.57
1:A:1082:LEU:O	1:A:1086:GLY:N	2.37	0.57
1:A:33:ALA:HB3	1:A:62:HIS:HA	1.87	0.56
1:A:454:ALA:HA	1:A:956:LEU:HD22	1.88	0.55
1:B:33:ALA:HB3	1:B:62:HIS:HA	1.88	0.55
1:B:1002:VAL:O	1:B:1006:ARG:NH1	2.36	0.55
1:A:561:ASP:HB2	1:B:561:ASP:HB2	1.89	0.54
1:A:785:GLY:HA3	1:A:985:SER:HB2	1.90	0.53
1:A:942:PHE:CZ	1:B:557:PRO:HB3	2.43	0.53
1:A:596:ARG:HG2	1:A:624:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:GLN:HG3	2:A:1101:B12:H472	1.91	0.53
1:A:251:SER:HB2	1:A:280:ALA:HB1	1.92	0.52
1:A:679:THR:HG21	4:A:1103:IVC:H40	1.91	0.52
1:B:738:GLU:OE2	1:B:742:GLN:NE2	2.41	0.52
1:A:228:GLU:OE1	1:A:232:ARG:NH1	2.43	0.52
1:B:572:GLU:HG2	1:B:581:THR:HG21	1.92	0.52
1:A:458:ARG:NH1	1:A:960:GLU:OE2	2.41	0.52
1:A:879:ASN:O	1:A:883:THR:OG1	2.26	0.51
1:A:265:ARG:NH1	5:A:1104:GDP:O1A	2.44	0.51
3:A:1102[A]:5AD:H5'1	4:A:1103:IVC:H43	1.92	0.51
1:B:785:GLY:HA3	1:B:985:SER:HB2	1.92	0.51
1:A:572:GLU:HG2	1:A:581:THR:HG21	1.93	0.51
1:A:916:ARG:NH1	1:B:875:GLU:OE2	2.44	0.51
2:A:1101:B12:H601	2:A:1101:B12:H252	1.94	0.50
1:B:879:ASN:O	1:B:883:THR:OG1	2.25	0.50
1:B:228:GLU:OE1	1:B:232:ARG:NH1	2.44	0.50
1:B:265:ARG:NH1	5:B:1103:GDP:O2A	2.44	0.50
1:B:30:VAL:HG23	1:B:78:VAL:HG11	1.93	0.50
1:A:30:VAL:HG23	1:A:78:VAL:HG11	1.93	0.49
1:A:697:ASP:OD1	1:A:1071:ARG:NH1	2.45	0.49
1:A:787:ASN:HB2	1:A:788:PRO:HD2	1.93	0.49
1:B:697:ASP:OD1	1:B:1071:ARG:NH1	2.45	0.49
1:A:513:LEU:HD21	1:A:566:LEU:HB2	1.94	0.49
1:B:787:ASN:HB2	1:B:788:PRO:HD2	1.94	0.49
1:A:296:ILE:O	1:A:300:LYS:HG3	2.13	0.49
1:B:296:ILE:O	1:B:300:LYS:HG3	2.13	0.49
1:B:731:VAL:O	1:B:733:ALA:N	2.47	0.48
1:A:734:ASP:O	1:A:737:LYS:HG2	2.13	0.48
1:B:513:LEU:HD21	1:B:566:LEU:HB2	1.94	0.48
1:B:267:ASN:HD21	1:B:1090:ARG:HA	1.78	0.48
1:A:250:PRO:HD3	1:A:312:SER:HB2	1.96	0.48
1:A:814:ASP:CG	1:A:854:ASN:HD22	2.17	0.48
1:B:458:ARG:NH1	1:B:960:GLU:OE2	2.43	0.48
1:B:866:THR:O	1:B:901:ASN:ND2	2.48	0.47
1:A:599:ALA:O	1:A:626:ALA:N	2.38	0.47
1:B:685:PRO:HB3	1:B:759:ILE:HD11	1.97	0.47
1:B:814:ASP:CG	1:B:854:ASN:HD22	2.17	0.47
1:A:780:HIS:CD2	4:A:1103:IVC:H44	2.50	0.47
1:A:49:ILE:HB	1:A:150:ILE:HG13	1.97	0.46
1:B:49:ILE:HB	1:B:150:ILE:HG13	1.97	0.46
1:B:141:GLY:HA3	2:B:1101:B12:H5R2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PRO:HD3	1:B:312:SER:HB2	1.97	0.46
1:A:779:TYR:CD2	1:A:825:SER:HB2	2.51	0.46
1:A:528:TYR:HB2	1:A:541:LEU:HD21	1.98	0.46
1:B:446:ARG:NH2	1:B:804:GLU:OE2	2.48	0.46
1:B:528:TYR:HB2	1:B:541:LEU:HD21	1.98	0.46
1:A:172:VAL:HG21	1:A:183:LEU:HD22	1.97	0.46
1:A:46:MET:SD	1:A:150:ILE:HD11	2.56	0.46
1:B:531:LYS:HA	1:B:536:GLU:HA	1.96	0.46
1:B:231:ARG:NH1	1:B:1084:GLU:HA	2.31	0.46
1:A:738:GLU:HB3	1:A:745:CYS:HB2	1.96	0.45
1:A:776:ILE:HD13	1:A:799:GLY:HA2	1.98	0.45
1:A:905:GLU:O	2:A:1101:B12:N29	2.38	0.45
1:B:731:VAL:HG23	1:B:771:PHE:HE1	1.80	0.45
1:A:902:ALA:HB1	1:A:914:SER:OG	2.16	0.45
1:B:902:ALA:HB1	1:B:914:SER:OG	2.17	0.45
1:A:598:PHE:HA	1:A:624:SER:HB3	1.99	0.45
2:A:1101:B12:H261	3:A:1102[B]:5AD:H2'	1.98	0.45
2:A:1101:B12:H463	4:A:1103:IVC:H43	1.99	0.45
1:B:599:ALA:HB3	1:B:611:PHE:CE1	2.52	0.45
2:A:1101:B12:H552	2:A:1101:B12:H531	1.99	0.45
1:B:46:MET:SD	1:B:150:ILE:HD11	2.57	0.45
1:B:172:VAL:HG21	1:B:183:LEU:HD22	1.98	0.45
1:B:731:VAL:HG23	1:B:771:PHE:CE1	2.52	0.45
1:A:657:LEU:HG	1:A:661:LYS:HE3	1.99	0.45
1:B:287:GLU:HG2	1:B:288:ILE:HG23	1.98	0.44
1:A:32:ALA:HB2	1:A:60:LEU:HB2	1.98	0.44
1:B:32:ALA:HB2	1:B:60:LEU:HB2	1.99	0.44
2:B:1101:B12:H363	2:B:1101:B12:H411	1.80	0.44
1:B:657:LEU:HG	1:B:661:LYS:HE3	1.99	0.44
1:A:685:PRO:HB3	1:A:759:ILE:HD11	1.99	0.44
1:A:62:HIS:CE1	1:A:743:ASN:HB3	2.52	0.44
1:A:597:MET:HB2	1:A:614:VAL:HG11	1.98	0.44
1:A:735:ILE:HG21	1:A:752:SER:HB2	1.99	0.44
1:A:866:THR:O	1:A:901:ASN:ND2	2.51	0.44
1:A:978:ARG:NE	1:A:1093:MET:OXT	2.45	0.43
1:A:453:LEU:HD21	1:A:851:TYR:CE2	2.53	0.43
1:A:584:VAL:HB	1:A:859:LYS:HB3	1.99	0.43
1:A:997:LEU:HD22	1:B:546:LEU:HD11	2.01	0.43
1:A:735:ILE:HA	1:A:738:GLU:HG2	2.01	0.43
2:B:1101:B12:H531	2:B:1101:B12:H552	2.00	0.43
1:A:681:ASN:HB2	1:A:744:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:B12:H253	2:B:1101:B12:H301	1.70	0.42
1:A:731:VAL:HG12	1:A:771:PHE:HE1	1.85	0.42
1:B:193:ASP:HA	1:B:194:PRO:HD3	1.94	0.42
1:A:757:GLY:HA3	1:A:809:ARG:NH2	2.34	0.42
1:A:999:ILE:N	1:A:1003:ASN:OD1	2.47	0.42
1:B:70:VAL:HG13	1:B:101:LEU:HD23	2.02	0.42
1:B:1056:VAL:HB	1:B:1085:VAL:HG21	2.01	0.42
1:A:70:VAL:HG13	1:A:101:LEU:HD23	2.02	0.42
1:A:87:GLN:O	1:A:650:SER:OG	2.38	0.42
1:A:114:GLY:HA3	2:A:1101:B12:C9B	2.49	0.42
1:B:200:LEU:HD11	1:B:298:ALA:HA	2.01	0.42
1:B:464:VAL:HG11	1:B:571:ARG:HG3	2.02	0.42
1:B:611:PHE:HB3	1:B:667:PHE:CZ	2.55	0.42
1:A:271:HIS:CG	1:A:272:PRO:HD2	2.55	0.41
1:B:160:ASP:OD2	1:B:162:THR:OG1	2.26	0.41
1:B:222:LYS:NZ	5:B:1103:GDP:O1B	2.42	0.41
1:B:271:HIS:CG	1:B:272:PRO:HD2	2.55	0.41
1:A:209:VAL:HA	1:A:210:PRO:HD3	1.88	0.41
1:A:778:GLY:HA3	1:A:795:THR:OG1	2.21	0.41
1:A:40:ASP:HA	1:A:43:ILE:HG22	2.03	0.41
1:A:222:LYS:NZ	5:A:1104:GDP:O1B	2.41	0.41
1:A:772:TYR:CZ	4:A:1103:IVC:H20	2.55	0.41
1:A:1000:ILE:N	1:B:928:GLU:OE2	2.42	0.41
1:B:42:SER:OG	2:B:1101:B12:N3B	2.50	0.41
2:B:1101:B12:H473	2:B:1101:B12:H481	1.81	0.41
1:A:580:TYR:CE1	1:A:859:LYS:HE2	2.56	0.41
1:B:526:ASP:HA	1:B:542:ILE:HG12	2.03	0.41
1:A:389:MET:HA	1:A:390:PRO:HD3	1.95	0.40
1:A:443:PRO:HA	1:A:444:PRO:HD3	1.89	0.40
1:A:464:VAL:HG11	1:A:571:ARG:HG3	2.02	0.40
1:A:737:LYS:O	1:A:741:GLY:N	2.47	0.40
1:B:358:LYS:HG2	5:B:1103:GDP:C6	2.56	0.40
1:A:829:ASP:HB2	1:A:832:TYR:CD2	2.55	0.40
1:B:1023:SER:HB3	1:B:1026:GLU:HG3	2.03	0.40
1:B:248:ILE:HD13	1:B:289:SER:H	1.87	0.40
1:B:829:ASP:HB2	1:B:832:TYR:CD2	2.57	0.40
1:A:358:LYS:HG2	5:A:1104:GDP:C6	2.56	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	1053/1113 (95%)	1009 (96%)	42 (4%)	2 (0%)	47	80
1	B	1051/1113 (94%)	1014 (96%)	34 (3%)	3 (0%)	41	75
All	All	2104/2226 (94%)	2023 (96%)	76 (4%)	5 (0%)	47	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	GLN
1	B	1091	ARG
1	A	489	HIS
1	B	319	ALA
1	A	741	GLY

### 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	823/906 (91%)	818 (99%)	5 (1%)	86	95
1	B	817/906 (90%)	815 (100%)	2 (0%)	93	98
All	All	1640/1812 (90%)	1633 (100%)	7 (0%)	91	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ASP

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Mol	Chain	Res	Type
1	A	598	PHE
1	A	744	THR
1	A	883	THR
1	A	1092	ASN
1	B	249	ASP
1	B	883	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	865	GLN
1	B	899	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	B12	B	1101	1	90,101,101	0.82	4 (4%)	137,166,166	1.00	9 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  >
5	GDP	B	1103	6	24,30,30	2.75	11 (45%)	30,47,47	1.32	5 (16%)
3	5AD	A	1102[B]	2	17,20,20	0.65	0	15,30,30	0.77	1 (6%)
4	IVC	B	1102	-	26,29,56	0.68	0	31,45,83	0.81	2 (6%)
4	IVC	A	1103	-	47,56,56	0.59	0	59,83,83	0.61	1 (1%)
2	B12	A	1101	1,3	90,101,101	0.83	5 (5%)	137,166,166	1.06	9 (6%)
5	GDP	A	1104	6	24,30,30	2.72	11 (45%)	30,47,47	1.32	5 (16%)
3	5AD	A	1102[A]	-	17,20,20	0.64	0	15,30,30	0.88	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B12	B	1101	1	-	12/52/223/223	0/3/11/11
5	GDP	B	1103	6	-	0/12/32/32	0/3/3/3
3	5AD	A	1102[B]	2	-	0/0/20/20	0/3/3/3
4	IVC	B	1102	-	-	3/11/31/71	0/3/3/3
4	IVC	A	1103	-	-	15/51/71/71	0/3/3/3
2	B12	A	1101	1,3	-	16/52/223/223	0/3/11/11
5	GDP	A	1104	6	-	0/12/32/32	0/3/3/3
3	5AD	A	1102[A]	-	-	0/0/20/20	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1103	GDP	O6-C6	6.78	1.37	1.23
5	A	1104	GDP	O6-C6	6.74	1.37	1.23
5	B	1103	GDP	C2-N2	5.95	1.48	1.34
5	A	1104	GDP	C2-N2	5.93	1.48	1.34
2	B	1101	B12	C14-N23	4.37	1.40	1.35
2	A	1101	B12	C14-N23	4.30	1.40	1.35
5	A	1104	GDP	C5-C4	-3.92	1.33	1.43
5	B	1103	GDP	C5-C4	-3.92	1.33	1.43
5	A	1104	GDP	O5'-C5'	-3.90	1.29	1.44
5	B	1103	GDP	O5'-C5'	-3.89	1.29	1.44
5	A	1104	GDP	C2-N1	-3.81	1.28	1.37
5	B	1103	GDP	C2-N1	-3.79	1.28	1.37
5	B	1103	GDP	C2'-C1'	-3.32	1.48	1.53
2	B	1101	B12	C16-C15	3.14	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	GDP	C2'-C1'	-3.12	1.49	1.53
5	B	1103	GDP	C2'-C3'	-2.71	1.45	1.53
2	A	1101	B12	C16-C15	2.67	1.52	1.44
5	A	1104	GDP	C2'-C3'	-2.67	1.46	1.53
5	B	1103	GDP	PA-O2A	-2.66	1.42	1.55
2	A	1101	B12	C9-N22	2.65	1.37	1.30
5	A	1104	GDP	C2-N3	2.47	1.39	1.33
5	B	1103	GDP	C2-N3	2.46	1.39	1.33
2	B	1101	B12	C1P-C2P	2.40	1.57	1.51
2	A	1101	B12	C1P-C2P	2.35	1.57	1.51
5	A	1104	GDP	PA-O1A	-2.27	1.42	1.50
2	B	1101	B12	C9-N22	2.20	1.36	1.30
5	B	1103	GDP	PB-O3B	-2.17	1.46	1.54
5	A	1104	GDP	PB-O3B	-2.14	1.46	1.54
5	A	1104	GDP	C6-N1	-2.07	1.34	1.37
5	B	1103	GDP	C6-N1	-2.05	1.34	1.37
2	A	1101	B12	C11-N23	-2.00	1.33	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	B12	C19-C1-N21	3.44	105.69	102.16
2	A	1101	B12	C30-C3-C2	-3.35	112.00	119.09
5	A	1104	GDP	C5-C6-N1	3.30	119.77	113.95
5	B	1103	GDP	C5-C6-N1	3.25	119.68	113.95
2	B	1101	B12	C30-C3-C2	-3.06	112.61	119.09
5	B	1103	GDP	PA-O3A-PB	-2.89	122.92	132.83
5	A	1104	GDP	PA-O3A-PB	-2.86	123.01	132.83
2	A	1101	B12	C8-C9-C10	-2.71	117.47	123.32
5	B	1103	GDP	C2-N1-C6	-2.71	120.11	125.10
2	B	1101	B12	C10-C9-N22	2.71	128.84	125.73
5	A	1104	GDP	C2-N1-C6	-2.69	120.14	125.10
5	B	1103	GDP	C8-N7-C5	2.65	108.04	102.99
4	B	1102	IVC	O4-P2-O10	2.64	113.87	106.47
5	A	1104	GDP	C8-N7-C5	2.61	107.96	102.99
2	A	1101	B12	C15-C16-N24	-2.49	118.83	122.42
2	B	1101	B12	C15-C16-N24	-2.48	118.84	122.42
2	B	1101	B12	C8-C9-C10	-2.48	117.97	123.32
5	A	1104	GDP	O6-C6-C5	-2.43	119.63	124.37
2	A	1101	B12	C10-C9-N22	2.40	128.48	125.73
2	B	1101	B12	C55-C17-C18	-2.37	106.57	111.15
4	B	1102	IVC	C8-C12-N5	2.33	123.90	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1103	GDP	O6-C6-C5	-2.31	119.86	124.37
2	A	1101	B12	C2-C1-C19	-2.28	115.00	118.60
4	A	1103	IVC	C8-C12-N5	2.28	123.82	120.35
2	A	1101	B12	C20-C1-C19	-2.27	107.16	109.36
3	A	1102[A]	5AD	C5-C6-N6	2.26	123.79	120.35
3	A	1102[B]	5AD	C5-C6-N6	2.22	123.73	120.35
2	B	1101	B12	C20-C1-C19	-2.21	107.23	109.36
2	B	1101	B12	C35-C5-C6	2.17	125.89	122.43
2	B	1101	B12	C35-C5-C4	-2.17	112.38	116.79
2	A	1101	B12	C30-C3-C4	2.16	114.66	109.63
2	A	1101	B12	C2-C1-N21	2.03	104.59	101.77
2	B	1101	B12	P-O2-C3R	2.01	126.73	119.41

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	B12	C18-C60-C61-N62
2	A	1101	B12	C1P-C2P-O3-P
2	A	1101	B12	C3P-C2P-O3-P
2	B	1101	B12	C2-C3-C30-C31
4	A	1103	IVC	C5-O4-P2-O12
4	A	1103	IVC	C5-O4-P2-O10
4	A	1103	IVC	C11-O8-P3-O14
4	A	1103	IVC	C11-O8-P3-O13
4	B	1102	IVC	C5-O4-P2-O12
4	B	1102	IVC	C5-O4-P2-O10
4	B	1102	IVC	C5-O4-P2-O7
2	A	1101	B12	C42-C41-C8-C9
2	B	1101	B12	C4-C3-C30-C31
2	A	1101	B12	C2-C3-C30-C31
2	A	1101	B12	C4-C3-C30-C31
4	A	1103	IVC	C2-C1-O2-P1
4	A	1103	IVC	C3-C1-O2-P1
2	B	1101	B12	C12-C13-C48-C49
2	B	1101	B12	C18-C60-C61-N62
2	B	1101	B12	C41-C42-C43-O44
2	A	1101	B12	C2P-O3-P-O4
2	A	1101	B12	C2P-O3-P-O5
2	B	1101	B12	C41-C42-C43-N45
2	A	1101	B12	C18-C60-C61-O63
2	B	1101	B12	C18-C60-C61-O63

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Mol	Chain	Res	Type	Atoms
2	B	1101	B12	C3R-O2-P-O3
4	A	1103	IVC	C22-C23-C24-C25
2	A	1101	B12	N59-C1P-C2P-O3
2	B	1101	B12	C55-C56-C57-O58
2	A	1101	B12	C55-C56-C57-O58
2	B	1101	B12	C55-C56-C57-N59
4	A	1103	IVC	P3-O7-P2-O12
2	A	1101	B12	C55-C56-C57-N59
4	A	1103	IVC	C20-C21-S1-C22
2	A	1101	B12	C12-C13-C48-C49
2	A	1101	B12	C38-C37-C7-C36
2	B	1101	B12	C38-C37-C7-C36
4	A	1103	IVC	C1-O2-P1-O5
4	A	1103	IVC	C1-O2-P1-O9
4	A	1103	IVC	C1-O2-P1-O6
4	A	1103	IVC	C5-O4-P2-O7
4	A	1103	IVC	C11-O8-P3-O7
2	B	1101	B12	C14-C13-C48-C49
4	A	1103	IVC	P3-O7-P2-O10
2	A	1101	B12	C30-C31-C32-O34
2	A	1101	B12	C30-C31-C32-N33

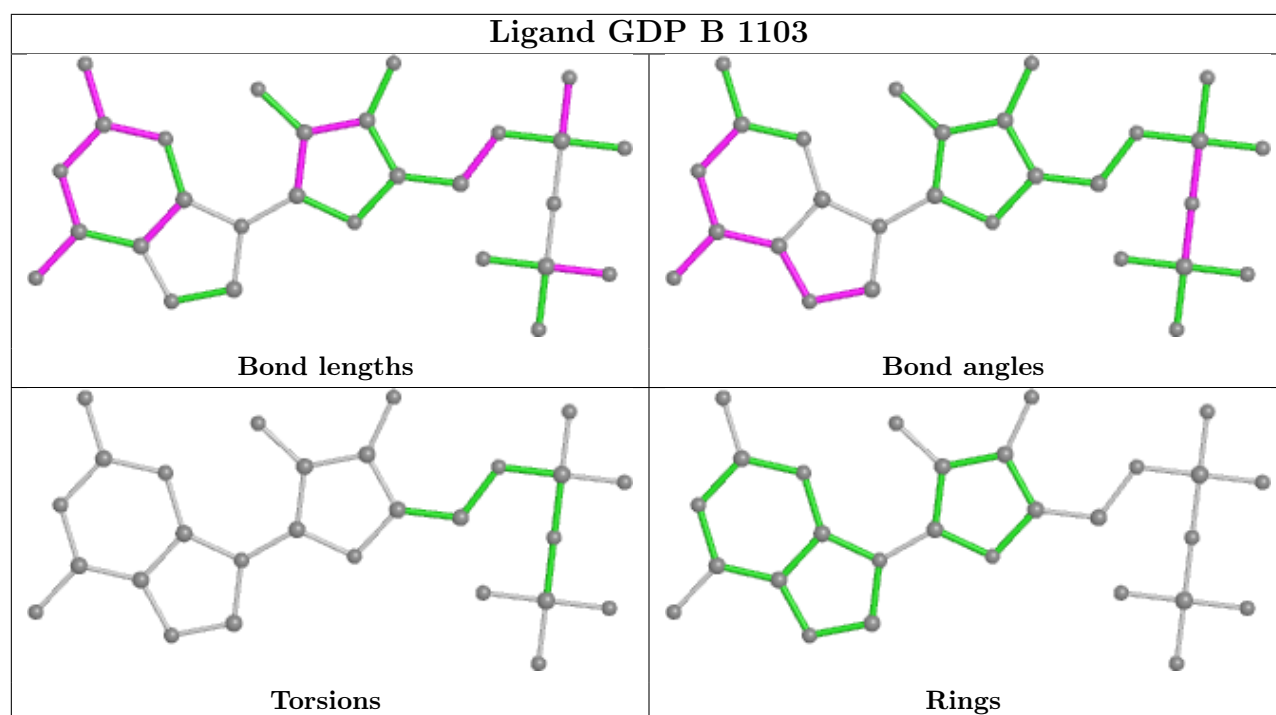
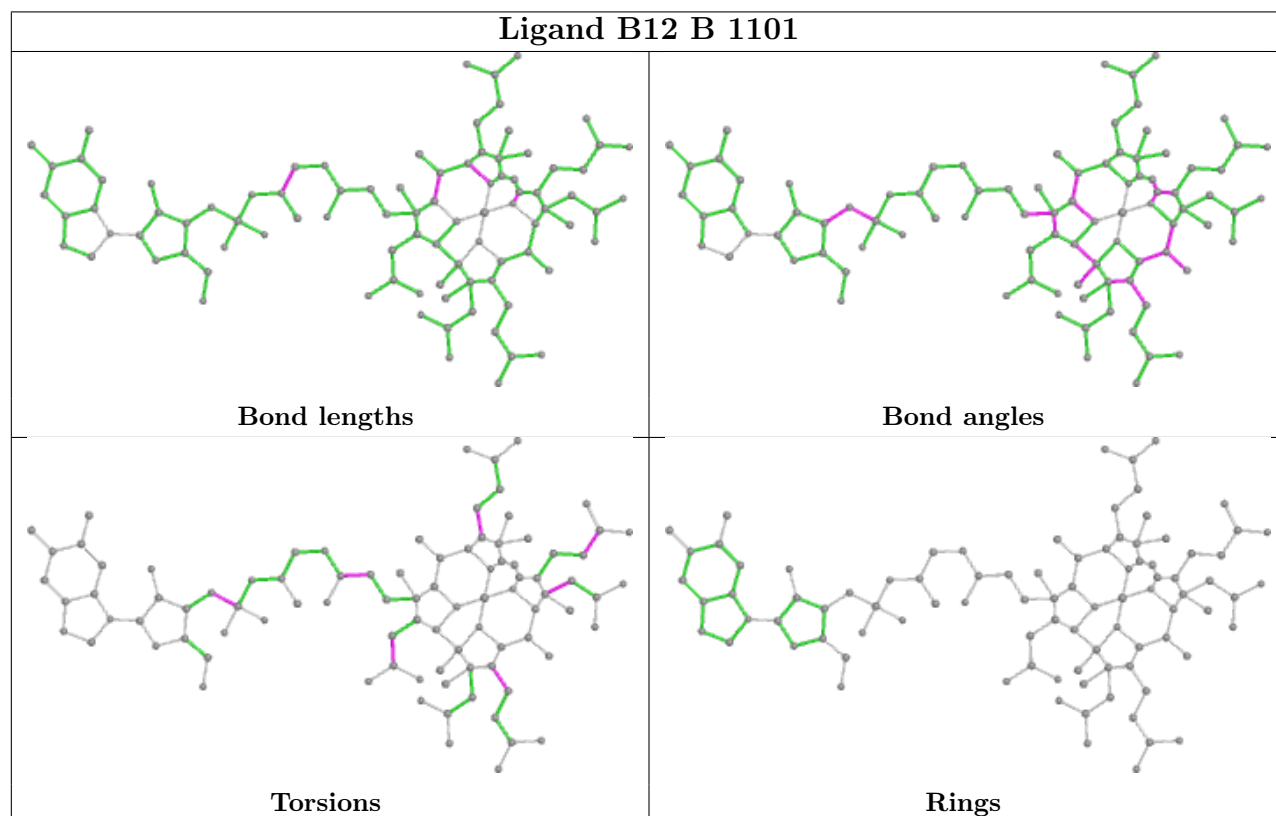
There are no ring outliers.

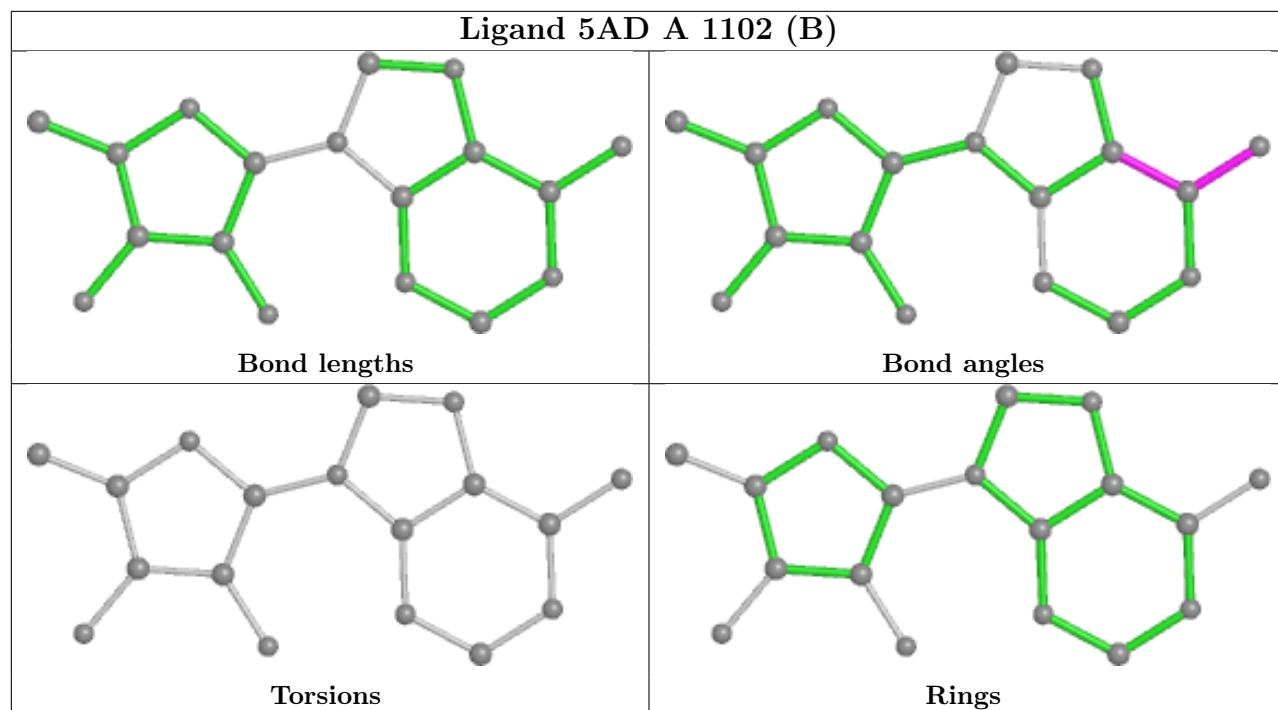
7 monomers are involved in 29 short contacts:

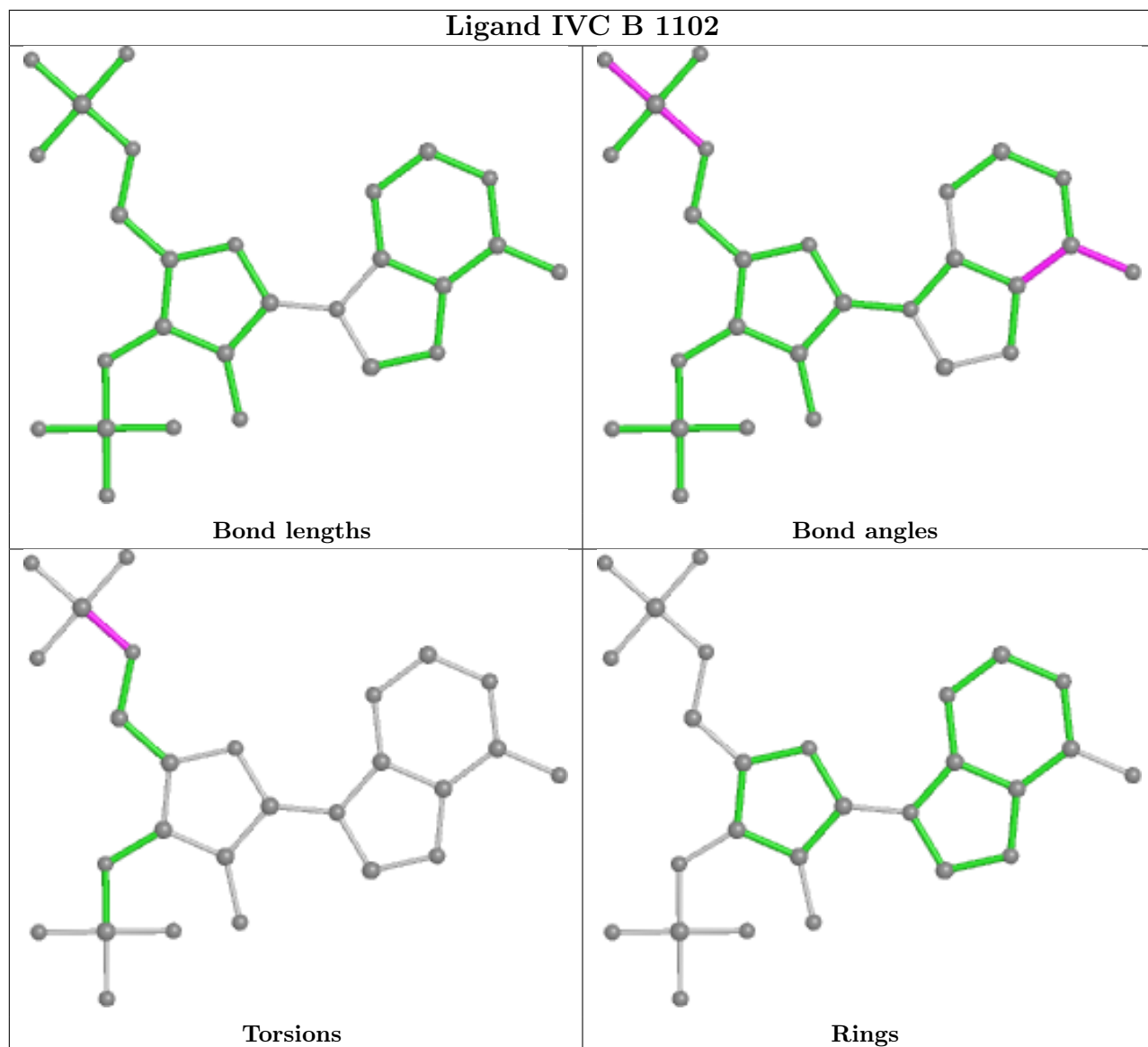
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	B12	6	0
5	B	1103	GDP	3	0
3	A	1102[B]	5AD	2	0
4	A	1103	IVC	7	0
2	A	1101	B12	10	0
5	A	1104	GDP	3	0
3	A	1102[A]	5AD	1	0

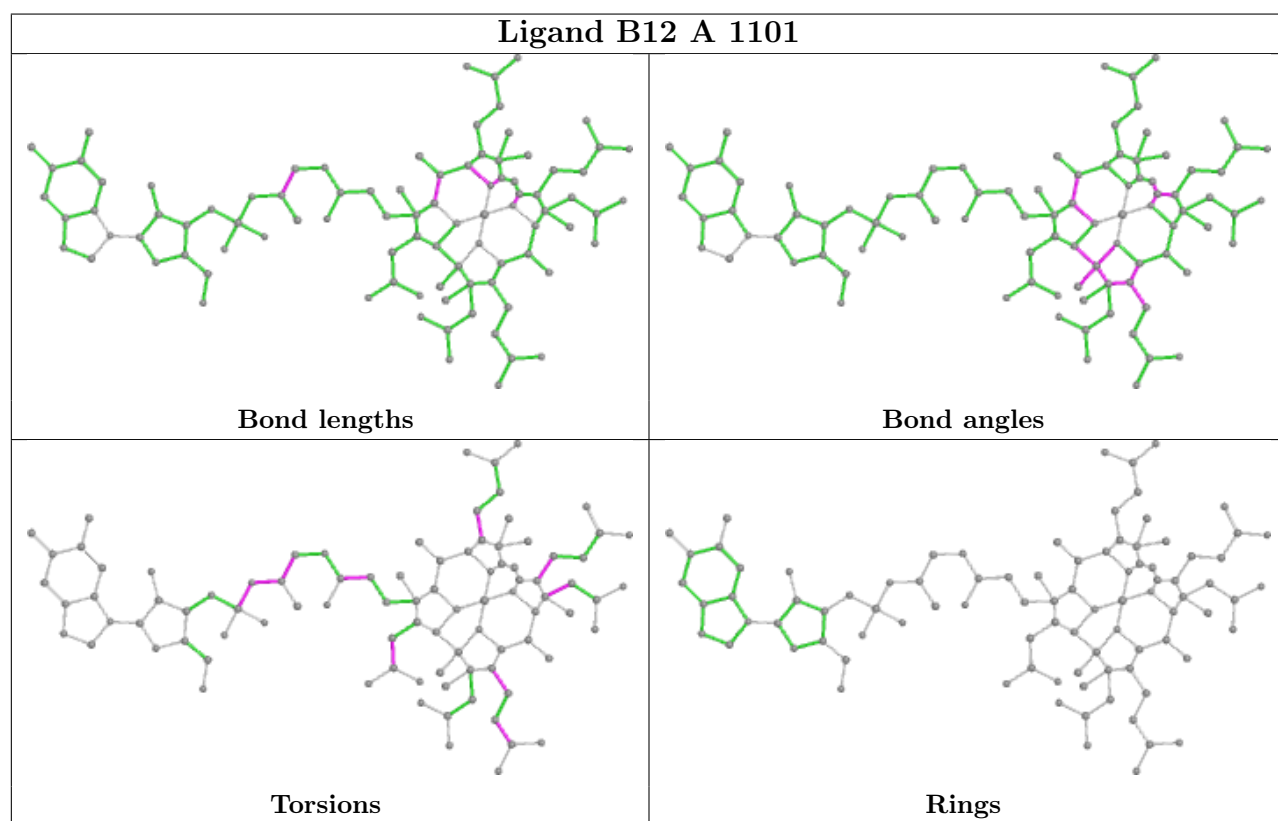
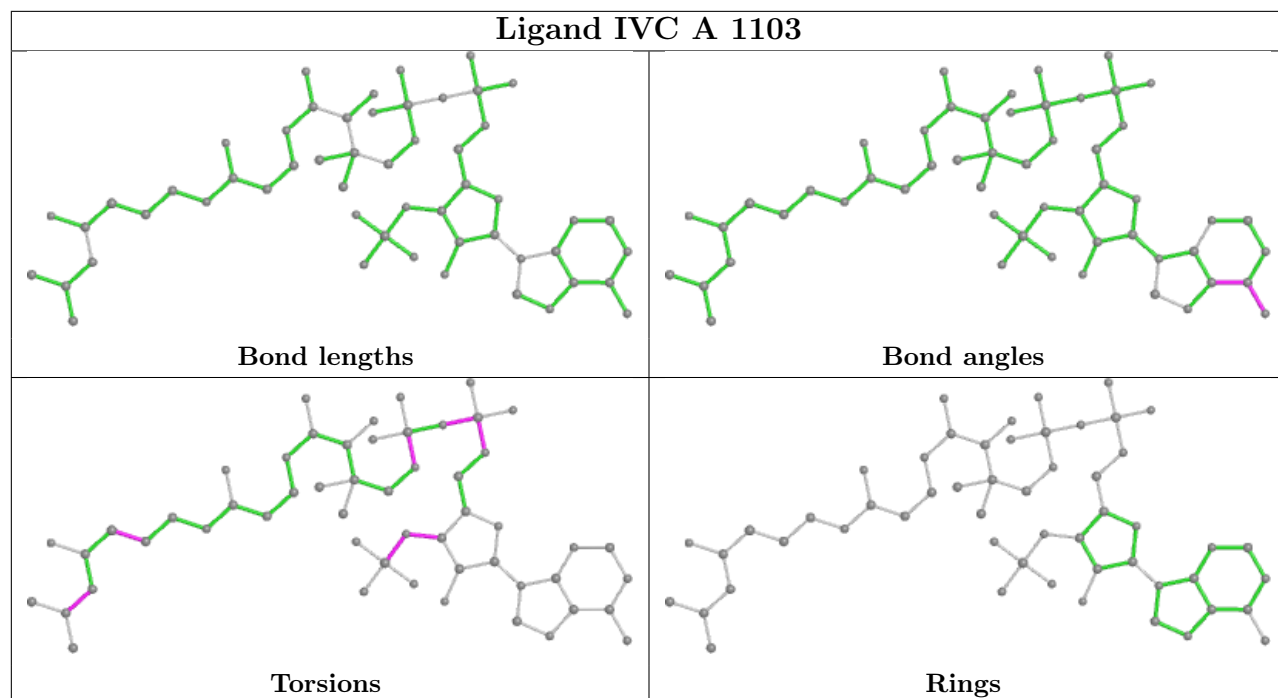
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

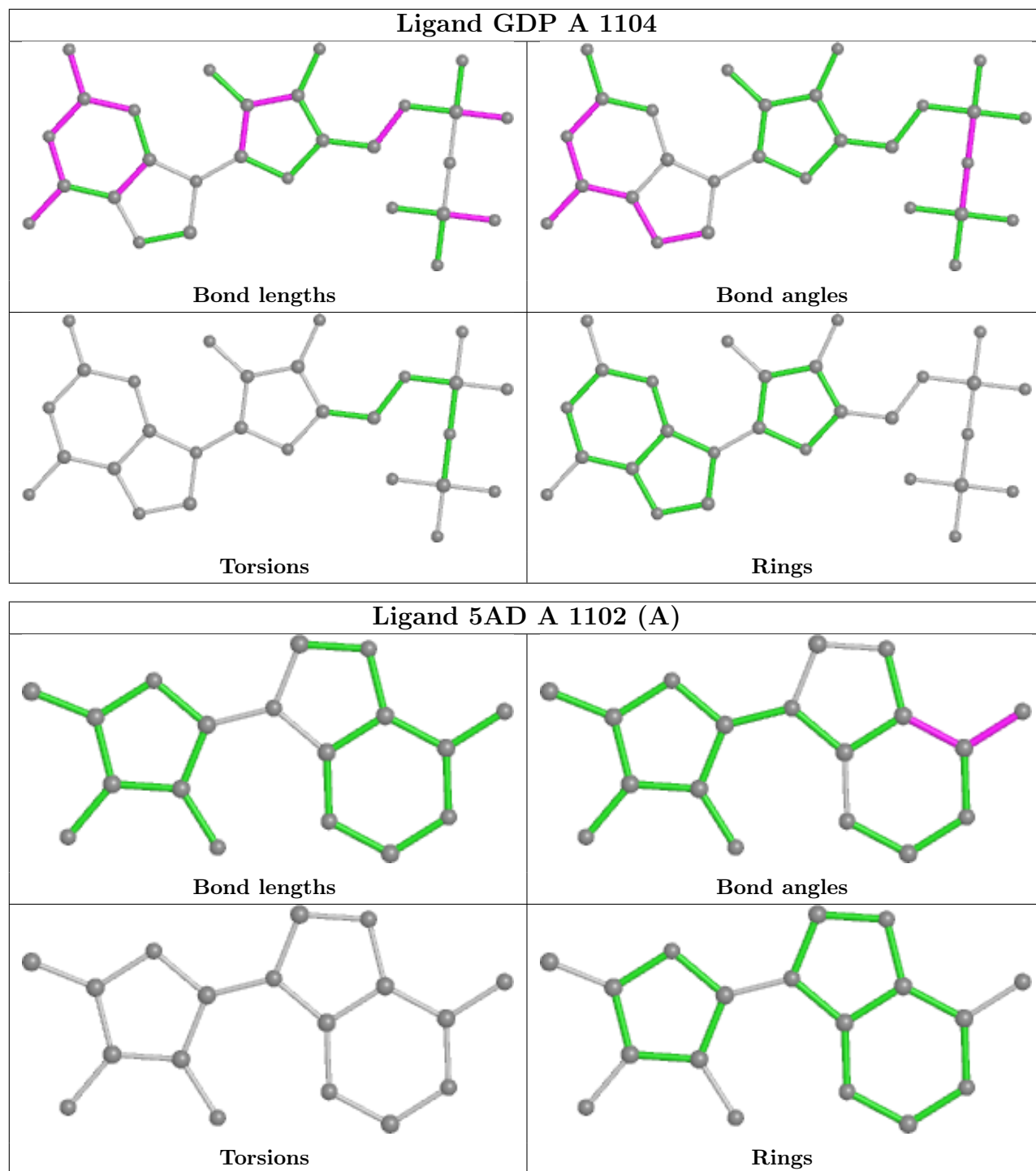












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1061/1113 (95%)	-0.08	14 (1%) 77 73	58, 88, 139, 180	0
1	B	1059/1113 (95%)	-0.11	22 (2%) 63 61	55, 82, 137, 212	0
All	All	2120/2226 (95%)	-0.09	36 (1%) 70 67	55, 85, 139, 212	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	909	THR	5.5
1	B	908	THR	4.1
1	A	1011	ASP	3.7
1	B	907	ILE	3.6
1	A	489	HIS	3.5
1	A	255	SER	3.3
1	A	420	MET	3.3
1	A	528	TYR	3.3
1	A	537	ILE	3.1
1	A	1015	GLN	2.9
1	A	316	GLN	2.8
1	B	1020	ALA	2.7
1	A	317	GLY	2.7
1	B	874	GLN	2.6
1	A	808	ALA	2.6
1	B	536	GLU	2.6
1	B	534	ASP	2.6
1	B	23	PRO	2.5
1	B	902	ALA	2.5
1	B	494	LEU	2.5
1	A	677	SER	2.4
1	B	1019	LEU	2.4
1	A	254	LYS	2.3
1	B	707	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	537	ILE	2.3
1	B	903	TYR	2.2
1	B	595	THR	2.2
1	B	706	ASP	2.2
1	B	872	HIS	2.2
1	B	530	VAL	2.1
1	A	1010	GLY	2.1
1	B	533	ARG	2.1
1	B	620	ALA	2.0
1	B	901	ASN	2.0
1	A	707	ASN	2.0
1	B	538	ARG	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 monosaccharides 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.

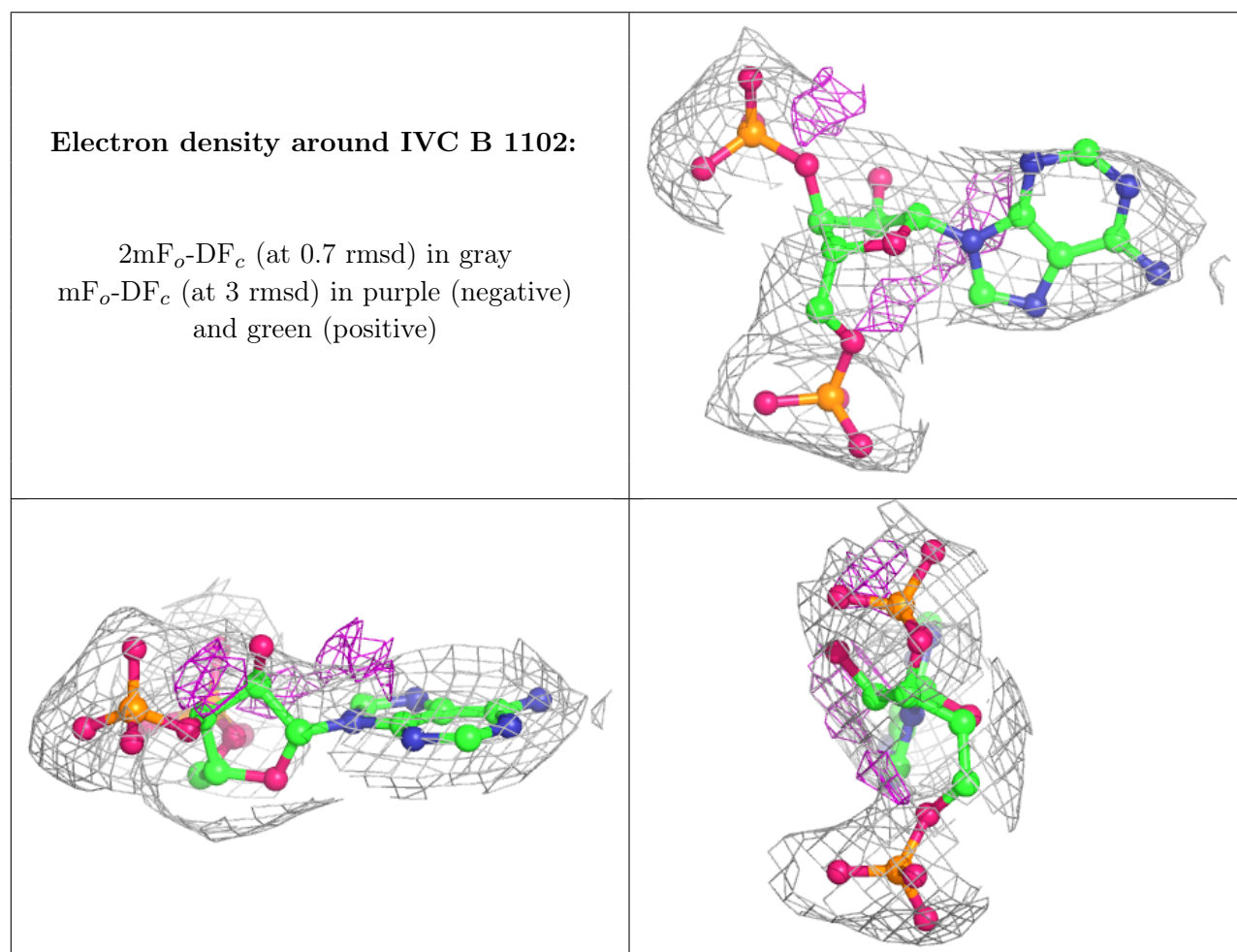
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	IVC	B	1102	27/54	0.83	0.27	130,147,183,185	0
4	IVC	A	1103	54/54	0.91	0.22	76,114,161,164	0
3	5AD	A	1102[B]	18/18	0.93	0.23	108,113,115,115	18
2	B12	B	1101	91/91	0.93	0.25	91,113,136,139	0
3	5AD	A	1102[A]	18/18	0.93	0.23	107,112,115,115	18
6	MG	A	1106	1/1	0.94	0.28	78,78,78,78	0
5	GDP	B	1103	28/28	0.95	0.19	55,65,72,123	0
5	GDP	A	1104	28/28	0.96	0.16	70,89,96,98	0
2	B12	A	1101	91/91	0.97	0.19	51,65,80,83	0
6	MG	A	1105	1/1	0.98	0.29	64,64,64,64	0
6	MG	B	1105	1/1	0.98	0.31	43,43,43,43	0

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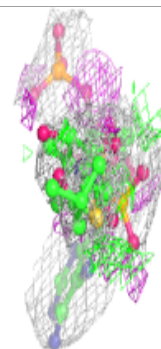
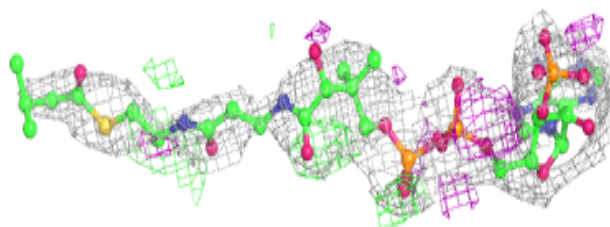
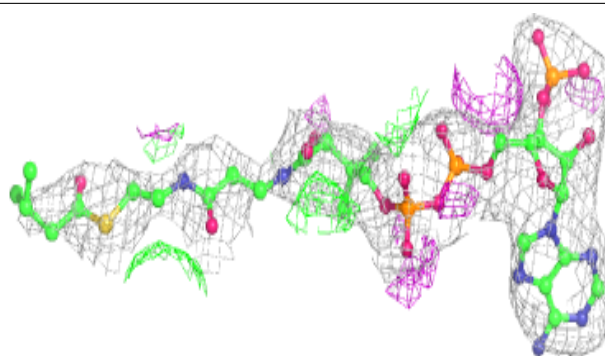
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	B	1104	1/1	0.99	0.28	42,42,42,42	0

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.

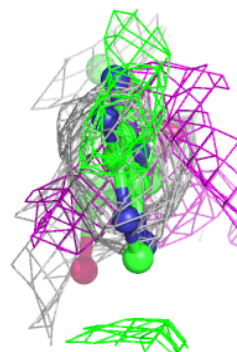
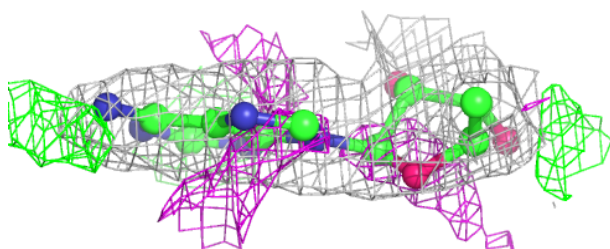
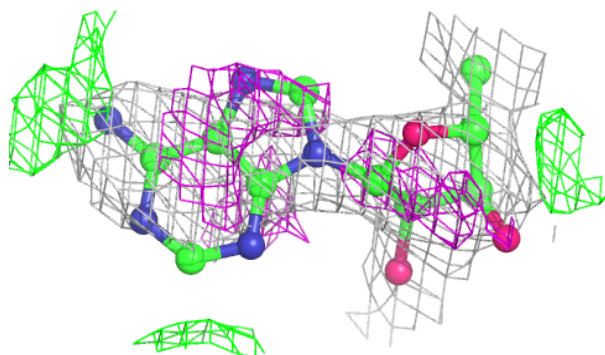


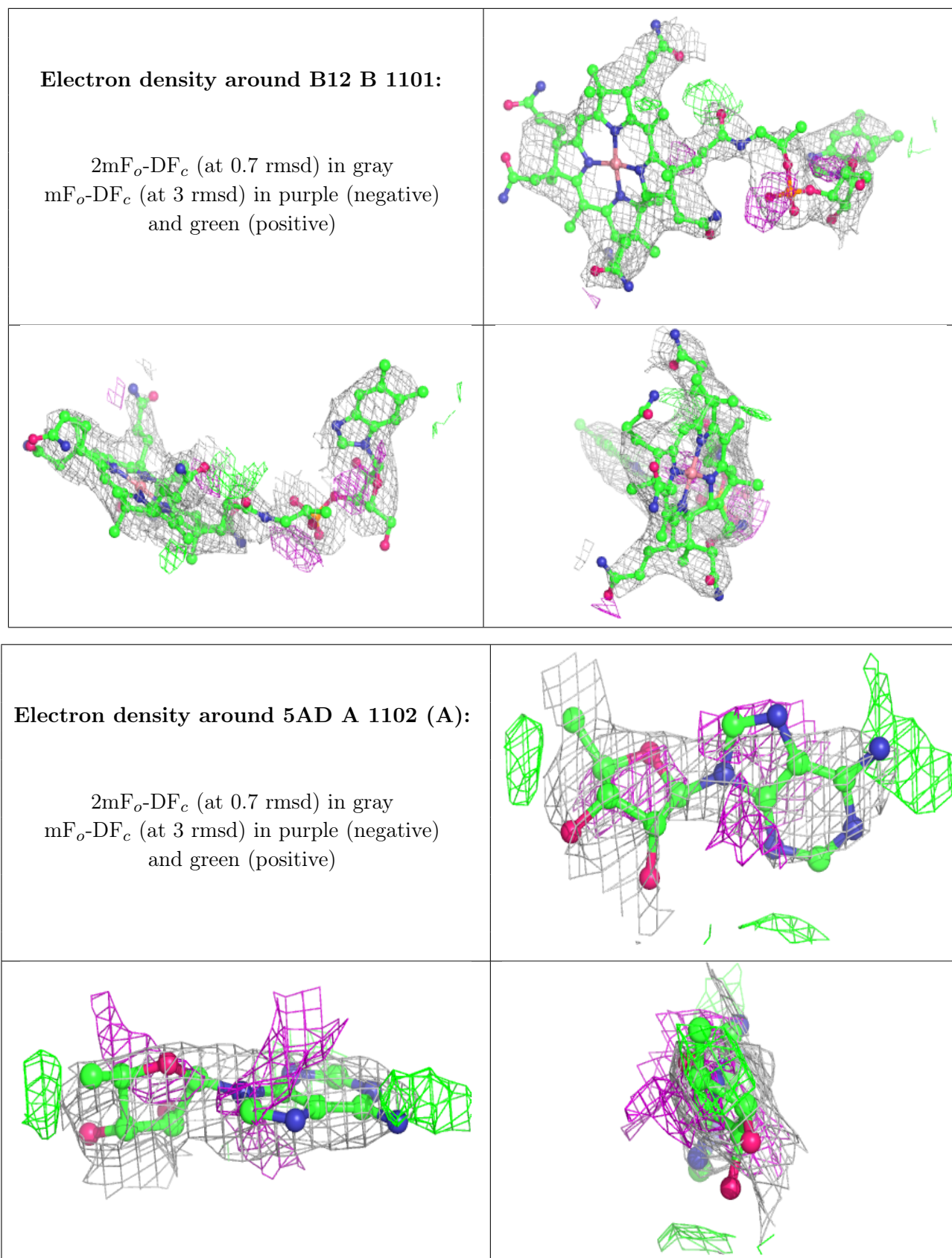
**Electron density around IVC A 1103:**

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

**Electron density around 5AD A 1102 (B):**

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

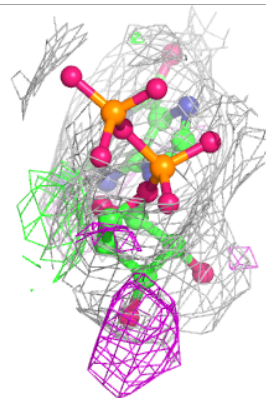
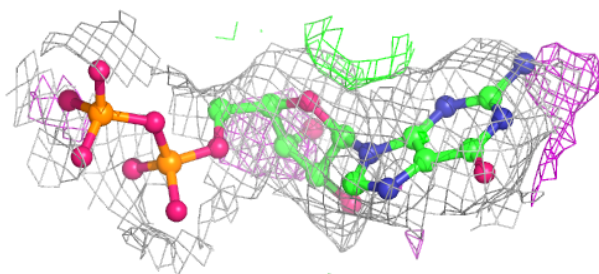
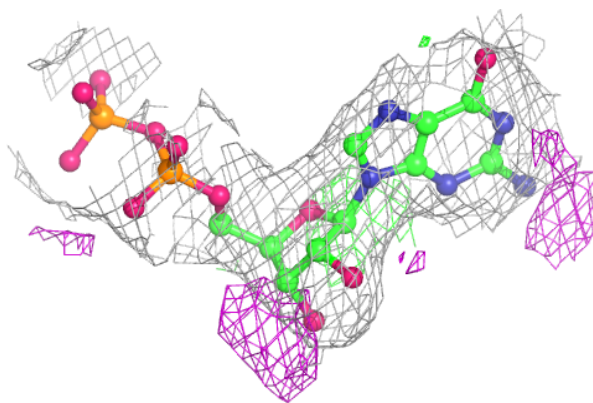




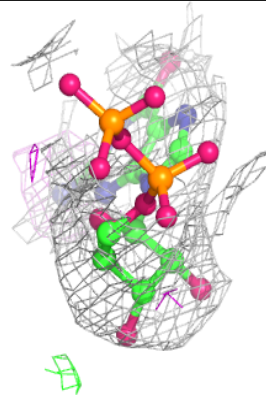
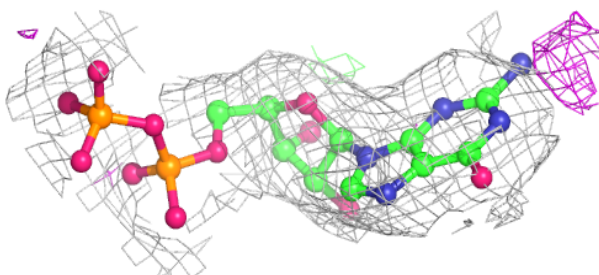
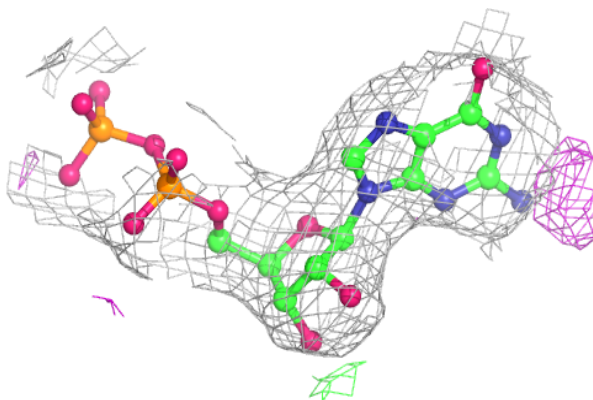


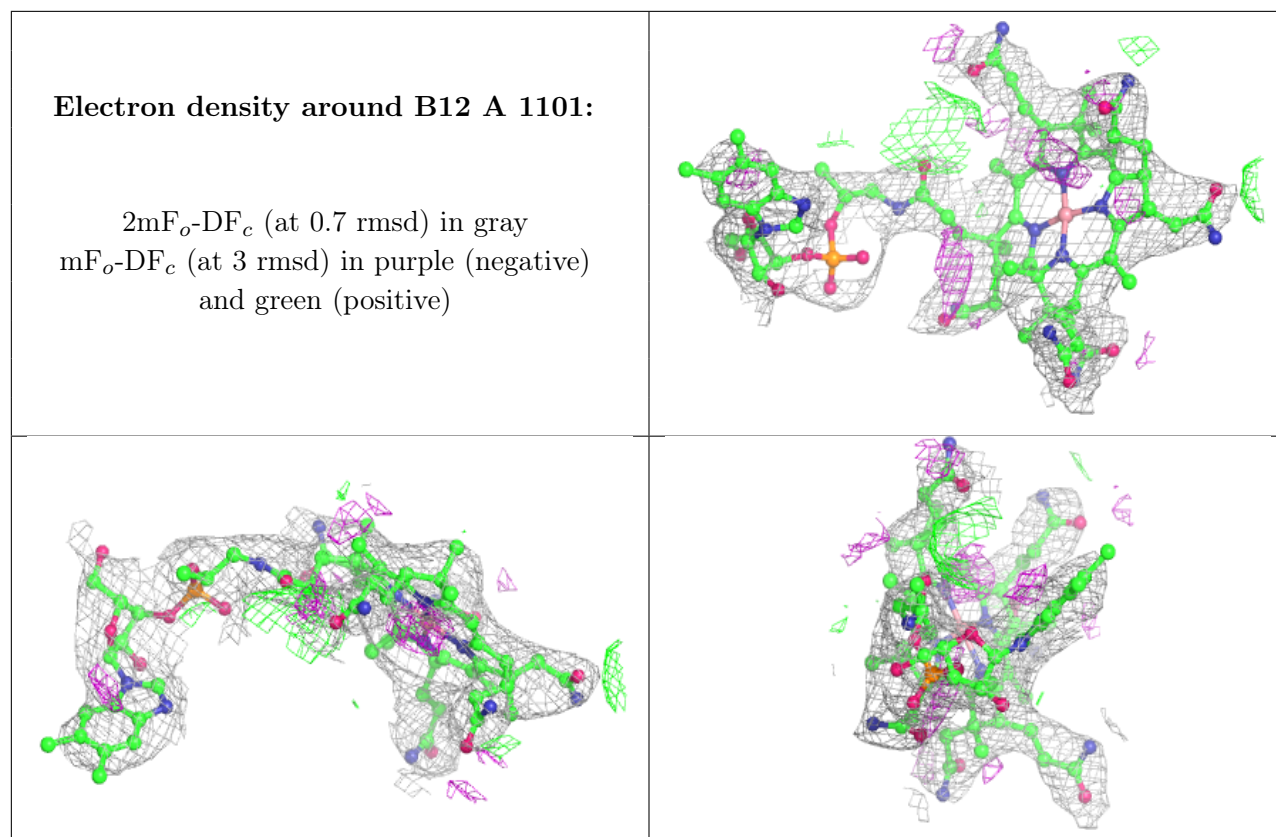
**Electron density around GDP B 1103:**

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

**Electron density around GDP A 1104:**

$2mF_o-DF_c$  (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.