



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:04 pm BST

PDB ID : 3DYH  
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-721  
Authors : Cao, R.; Gao, Y.; Robinson, H.; Goddard, A.; Oldfield, E.  
Deposited on : 2008-07-27  
Resolution : 1.94 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

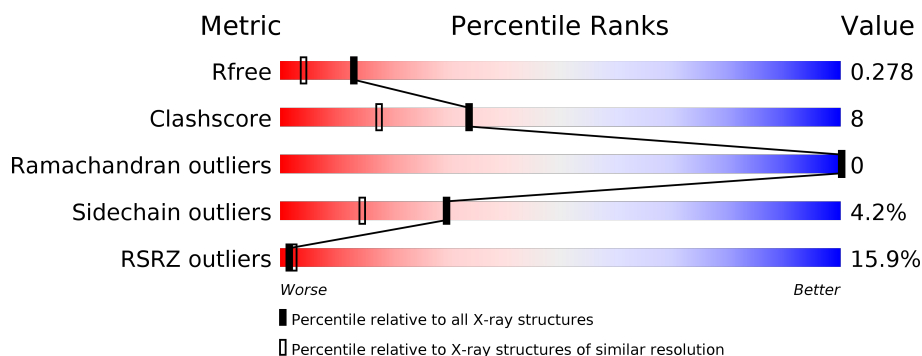
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	390	
1	B	390	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6133 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2864	1826	472	538	28			
1	B	359	Total	C	N	O	S	0	0	0
			2872	1830	474	540	28			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q86C09
A	-21	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-20	SER	-	EXPRESSION TAG	UNP Q86C09
A	-19	SER	-	EXPRESSION TAG	UNP Q86C09
A	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-12	SER	-	EXPRESSION TAG	UNP Q86C09
A	-11	SER	-	EXPRESSION TAG	UNP Q86C09
A	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
A	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
A	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
A	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
A	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-4	SER	-	EXPRESSION TAG	UNP Q86C09
A	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-2	MET	-	EXPRESSION TAG	UNP Q86C09
A	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
A	0	SER	-	EXPRESSION TAG	UNP Q86C09
B	-22	MET	-	EXPRESSION TAG	UNP Q86C09
B	-21	GLY	-	EXPRESSION TAG	UNP Q86C09

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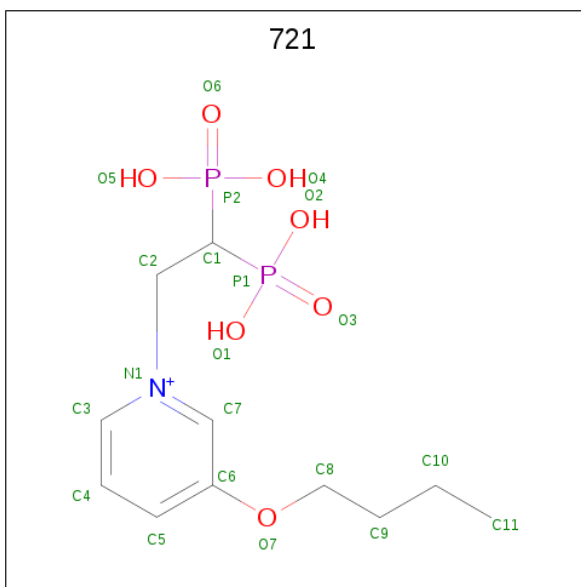
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP Q86C09
B	-19	SER	-	EXPRESSION TAG	UNP Q86C09
B	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-12	SER	-	EXPRESSION TAG	UNP Q86C09
B	-11	SER	-	EXPRESSION TAG	UNP Q86C09
B	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
B	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
B	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
B	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
B	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-4	SER	-	EXPRESSION TAG	UNP Q86C09
B	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-2	MET	-	EXPRESSION TAG	UNP Q86C09
B	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
B	0	SER	-	EXPRESSION TAG	UNP Q86C09

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is 3-butoxy-1-(2,2-diphosphonoethyl)pyridinium (three-letter code: 721) (formula: C<sub>11</sub>H<sub>20</sub>NO<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	11	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			21	11	1	7	2		

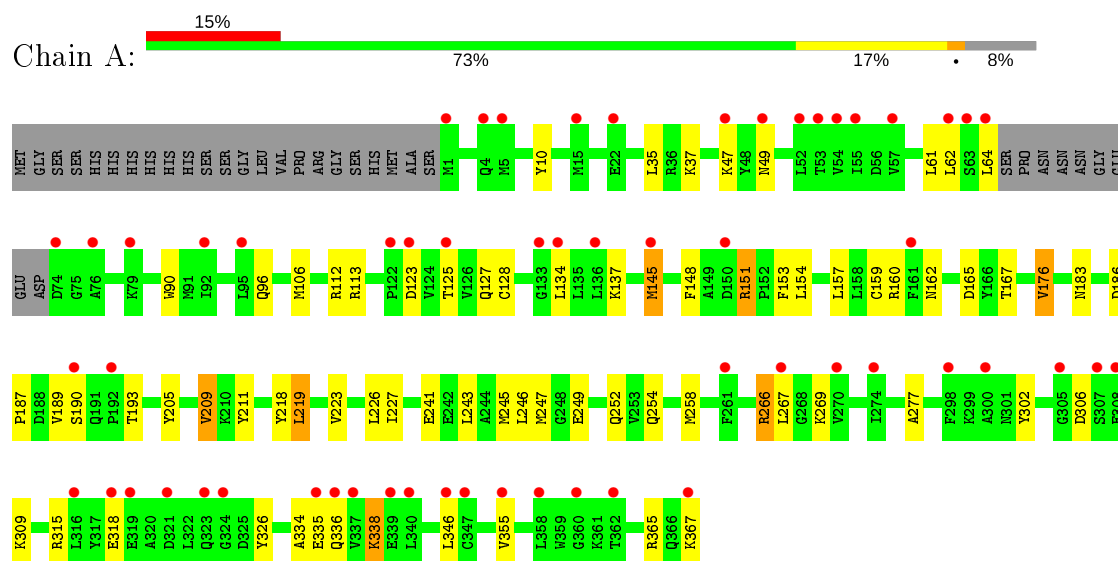
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	176	Total	O	0	0
			176	176		

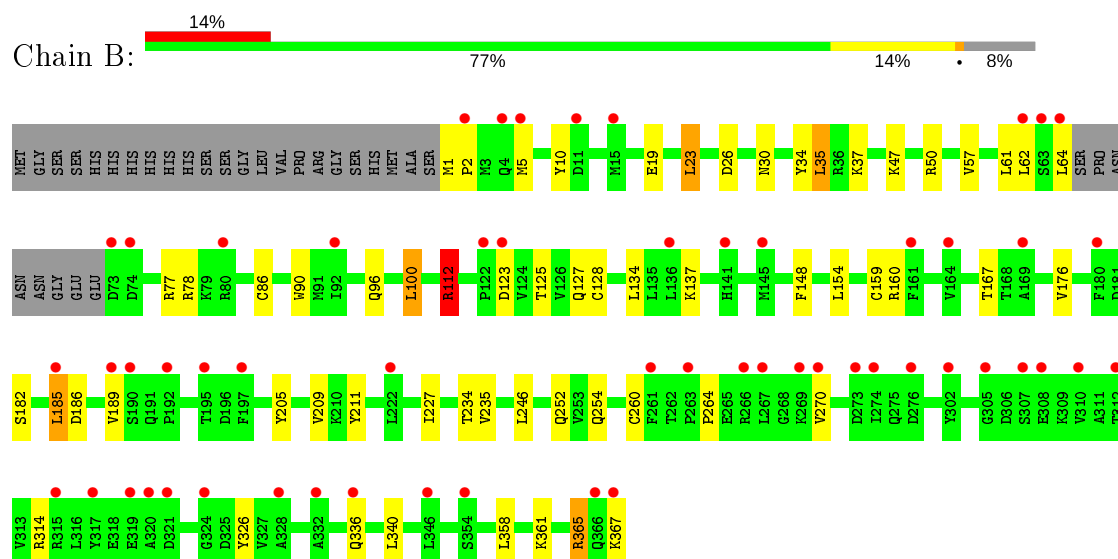
### 3 Residue-property plots [i](#)

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: Farnesyl pyrophosphate synthase



#### • Molecule 1: Farnesyl pyrophosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.91Å 118.73Å 63.04Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	28.83 – 1.94 28.83 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.83-1.94) 98.1 (28.83-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.282 0.238 , 0.278	Depositor DCC
$R_{free}$ test set	3331 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.53% 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, 721

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	0.53	0/2923	0.63	0/3952
1	B	0.55	0/2931	0.64	1/3963 (0.0%)
All	All	0.54	0/5854	0.64	1/7915 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	-6.55	117.02	120.30

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	2864	0	2824	61	0
1	B	2872	0	2830	44	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	21	0	16	0	0
3	B	21	0	16	1	0
4	A	173	0	0	9	0
4	B	176	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6133	0	5686	97	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 8.

All (97) 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:47:LYS:HD3	1:A:367:LYS:HD2	1.32	1.11
1:A:123:ASP:CB	1:B:186:ASP:O	2.03	1.07
1:B:112:ARG:NH2	3:B:4001:721:O2	2.01	0.94
1:A:137:LYS:HE2	1:A:165:ASP:OD2	1.69	0.92
1:A:134:LEU:HD21	4:B:4084:HOH:O	1.68	0.92
1:A:159:CYS:HB2	4:A:3176:HOH:O	1.69	0.91
1:A:186:ASP:O	1:B:123:ASP:CB	2.19	0.90
1:B:159:CYS:SG	4:B:4167:HOH:O	2.33	0.86
1:A:96:GLN:HG3	4:A:3171:HOH:O	1.75	0.85
1:B:134:LEU:HD21	4:B:4084:HOH:O	1.75	0.85
1:A:106:MET:O	4:A:3177:HOH:O	1.97	0.81
1:A:334:ALA:O	1:A:338:LYS:HE3	1.82	0.80
1:A:47:LYS:CD	1:A:367:LYS:HD2	2.12	0.79
1:A:218:TYR:CE2	1:A:247:MET:HE2	2.17	0.78
1:A:151:ARG:HG2	1:A:153:PHE:CZ	2.19	0.78
1:A:315:ARG:HA	1:A:318:GLU:HG2	1.68	0.75
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.71	0.73
1:A:266:ARG:HB2	1:A:266:ARG:NH1	2.05	0.72
1:A:162:ASN:ND2	4:A:3113:HOH:O	2.24	0.70
1:B:125:THR:HG23	4:B:4102:HOH:O	1.93	0.68
1:A:151:ARG:HG2	1:A:153:PHE:CE2	2.29	0.67
4:A:3177:HOH:O	1:B:127:GLN:HG3	2.01	0.60
1:A:209:VAL:HG22	1:A:252:GLN:CG	2.32	0.60
1:A:49:ASN:HD21	1:A:367:LYS:NZ	1.99	0.60
1:B:270:VAL:HA	4:B:4058:HOH:O	2.01	0.58
1:B:361:LYS:HE3	4:B:4118:HOH:O	2.03	0.58
1:B:50:ARG:NH1	1:B:96:GLN:OE1	2.37	0.57
1:B:160:ARG:HD2	1:B:227:ILE:HD11	1.85	0.56
1:A:189:VAL:O	1:B:123:ASP:CB	2.54	0.56
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.89	0.54
1:B:209:VAL:HG11	1:B:252:GLN:HB3	1.89	0.54
1:A:267:LEU:HD23	1:A:269:LYS:HG2	1.90	0.54
1:A:243:LEU:HD13	1:A:355:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD21	1:B:336:GLN:HB2	1.90	0.53
1:A:123:ASP:CB	1:B:189:VAL:O	2.56	0.53
1:A:176:VAL:CG2	1:B:127:GLN:HG3	2.38	0.53
1:B:19:GLU:O	1:B:23:LEU:HD23	2.09	0.53
1:B:96:GLN:NE2	4:B:4054:HOH:O	2.42	0.53
1:A:365:ARG:HB2	1:A:367:LYS:HG2	1.91	0.52
1:A:183:ASN:HD22	1:B:30:ASN:HD21	1.57	0.52
1:B:260:CYS:SG	1:B:314:ARG:HG2	2.50	0.51
1:A:125:THR:HB	1:A:127:GLN:OE1	2.11	0.50
1:A:61:LEU:HD11	1:A:226:LEU:HD23	1.94	0.50
1:B:100:LEU:HG	1:B:112:ARG:CZ	2.41	0.50
1:A:167:THR:HG23	1:A:211:TYR:HD1	1.77	0.49
1:B:264:PRO:HA	4:B:4058:HOH:O	2.12	0.49
1:B:254:GLN:HG2	1:B:326:TYR:OH	2.11	0.49
1:A:266:ARG:HB2	1:A:266:ARG:CZ	2.42	0.49
1:A:49:ASN:ND2	1:A:367:LYS:NZ	2.60	0.49
1:A:219:LEU:HD22	1:A:223:VAL:HG23	1.93	0.49
1:A:258:MET:HB3	1:A:267:LEU:HD11	1.94	0.49
1:A:61:LEU:CD1	1:A:226:LEU:HD23	2.43	0.48
1:A:246:LEU:HD21	1:A:336:GLN:HB2	1.95	0.48
1:B:64:LEU:HD13	1:B:234:THR:HG21	1.94	0.48
1:A:37:LYS:HG3	4:A:3107:HOH:O	2.12	0.48
1:B:167:THR:HG23	1:B:211:TYR:HD1	1.79	0.48
1:A:254:GLN:HG2	1:A:326:TYR:OH	2.14	0.47
1:B:148:PHE:HB2	1:B:154:LEU:HD13	1.96	0.47
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.50	0.47
1:A:266:ARG:HB2	1:A:266:ARG:HH11	1.79	0.47
1:A:112:ARG:HG3	1:A:113:ARG:HG3	1.96	0.47
1:A:218:TYR:HE2	1:A:247:MET:HE2	1.73	0.46
1:B:182:SER:O	1:B:185:LEU:HB2	2.15	0.46
1:B:361:LYS:NZ	4:B:4109:HOH:O	2.42	0.46
1:B:125:THR:HB	1:B:127:GLN:OE1	2.16	0.46
4:A:3065:HOH:O	1:B:26:ASP:HB2	2.16	0.46
1:B:57:VAL:O	1:B:61:LEU:HD23	2.16	0.46
1:B:209:VAL:CG1	1:B:252:GLN:HB3	2.45	0.45
1:B:127:GLN:HG2	1:B:128:CYS:N	2.32	0.45
1:A:148:PHE:HB2	1:A:154:LEU:HD13	1.98	0.45
1:A:49:ASN:HD21	1:A:367:LYS:HZ3	1.64	0.45
1:B:62:LEU:HD21	1:B:78:ARG:HG3	1.99	0.44
1:A:145:MET:HE2	1:B:159:CYS:HA	1.98	0.44
1:B:10:TYR:HB2	1:B:90:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HH11	1:A:367:LYS:HG3	1.83	0.44
1:B:47:LYS:HE3	4:B:4071:HOH:O	2.17	0.44
1:A:151:ARG:CG	1:A:153:PHE:CE2	3.00	0.44
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.53	0.43
1:A:365:ARG:HD2	1:A:367:LYS:HG2	2.00	0.43
1:B:205:TYR:CZ	1:B:209:VAL:HG21	2.54	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.01	0.43
1:A:96:GLN:CG	4:A:3171:HOH:O	2.50	0.43
1:A:306:ASP:HB3	1:A:309:LYS:HD2	2.01	0.42
1:A:96:GLN:NE2	4:A:3171:HOH:O	2.52	0.42
1:B:34:TYR:HD1	1:B:35:LEU:HD13	1.85	0.42
1:A:367:LYS:HA	1:A:367:LYS:HD3	1.82	0.42
1:B:96:GLN:HG3	4:B:4054:HOH:O	2.19	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.86	0.41
1:A:258:MET:HB3	1:A:267:LEU:CD1	2.50	0.41
1:A:49:ASN:ND2	1:A:367:LYS:HZ3	2.17	0.41
1:B:365:ARG:HH21	1:B:367:LYS:HG3	1.85	0.41
1:A:241:GLU:O	1:A:245:MET:HG2	2.20	0.41
1:A:127:GLN:HG2	1:A:128:CYS:N	2.35	0.41
1:A:209:VAL:CG1	1:A:249:GLU:HA	2.51	0.40
1:B:5:MET:HG2	1:B:86:CYS:SG	2.61	0.40
1:A:187:PRO:HG2	1:B:37:LYS:HG2	2.02	0.40
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.57	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	354/390 (91%)	346 (98%)	8 (2%)	0	100	100
1	B	355/390 (91%)	350 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	709/780 (91%)	696 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	311/340 (92%)	297 (96%)	14 (4%)	27	12
1	B	312/340 (92%)	300 (96%)	12 (4%)	33	18
All	All	623/680 (92%)	597 (96%)	26 (4%)	30	14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	64	LEU
1	A	145	MET
1	A	151	ARG
1	A	157	LEU
1	A	176	VAL
1	A	190	SER
1	A	193	THR
1	A	209	VAL
1	A	219	LEU
1	A	266	ARG
1	A	335	GLU
1	A	338	LYS
1	A	346	LEU
1	B	23	LEU
1	B	35	LEU
1	B	77	ARG
1	B	100	LEU
1	B	112	ARG
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	185	LEU
1	B	235	VAL
1	B	340	LEU
1	B	358	LEU
1	B	365	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	49	ASN
1	A	121	HIS
1	A	183	ASN
1	B	155	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](#)

Of 8 ligands modelled in this entry, 6 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
3	721	A	3001	2	20,21,21	1.07	0	25,30,30	1.15	3 (12%)
3	721	B	4001	2	20,21,21	1.17	2 (10%)	25,30,30	0.99	1 (4%)

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	721	A	3001	2	-	2/19/21/21	0/1/1/1
3	721	B	4001	2	-	2/19/21/21	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4001	721	P1-O2	-2.86	1.50	1.54
3	B	4001	721	P1-O1	-2.39	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	721	C2-N1-C7	-2.77	115.88	120.17
3	A	3001	721	O6-P2-C1	-2.65	104.78	112.29
3	B	4001	721	O3-P1-C1	-2.51	105.17	112.29
3	A	3001	721	C2-N1-C3	2.06	123.56	120.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

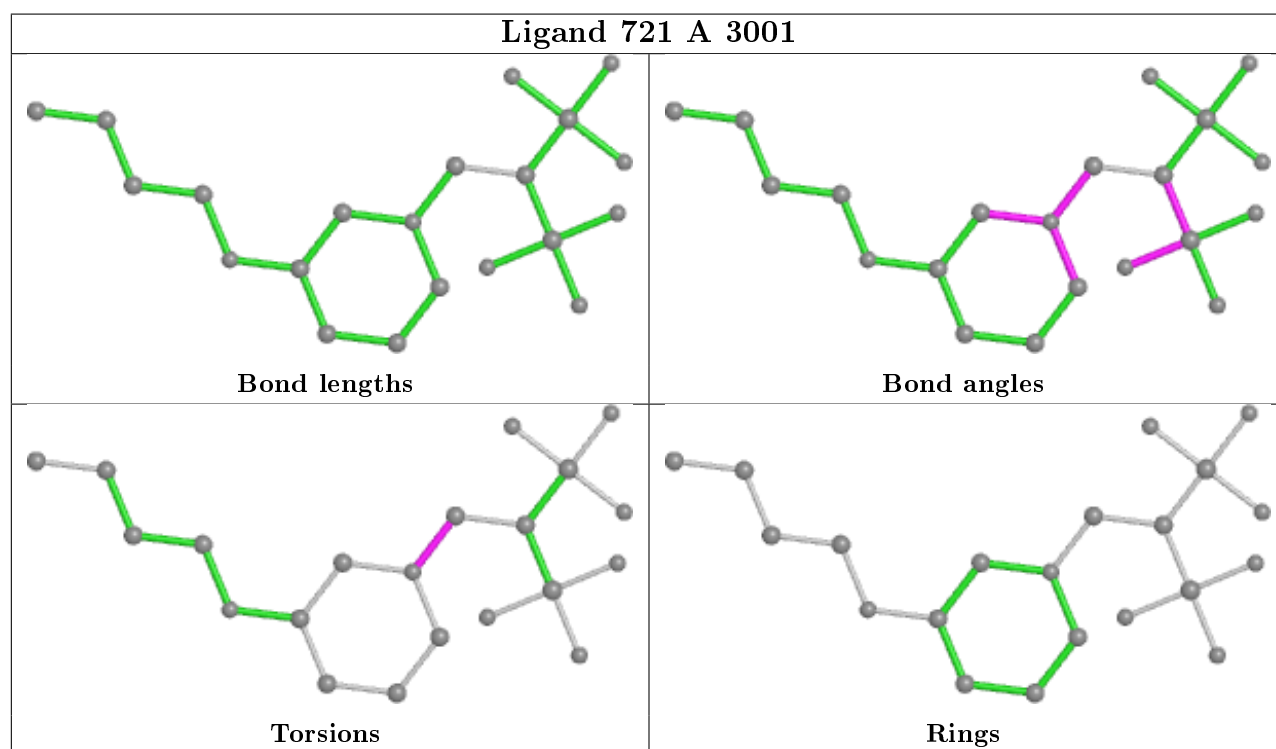
Mol	Chain	Res	Type	Atoms
3	A	3001	721	C1-C2-N1-C3
3	A	3001	721	C1-C2-N1-C7
3	B	4001	721	C1-C2-N1-C3
3	B	4001	721	C1-C2-N1-C7

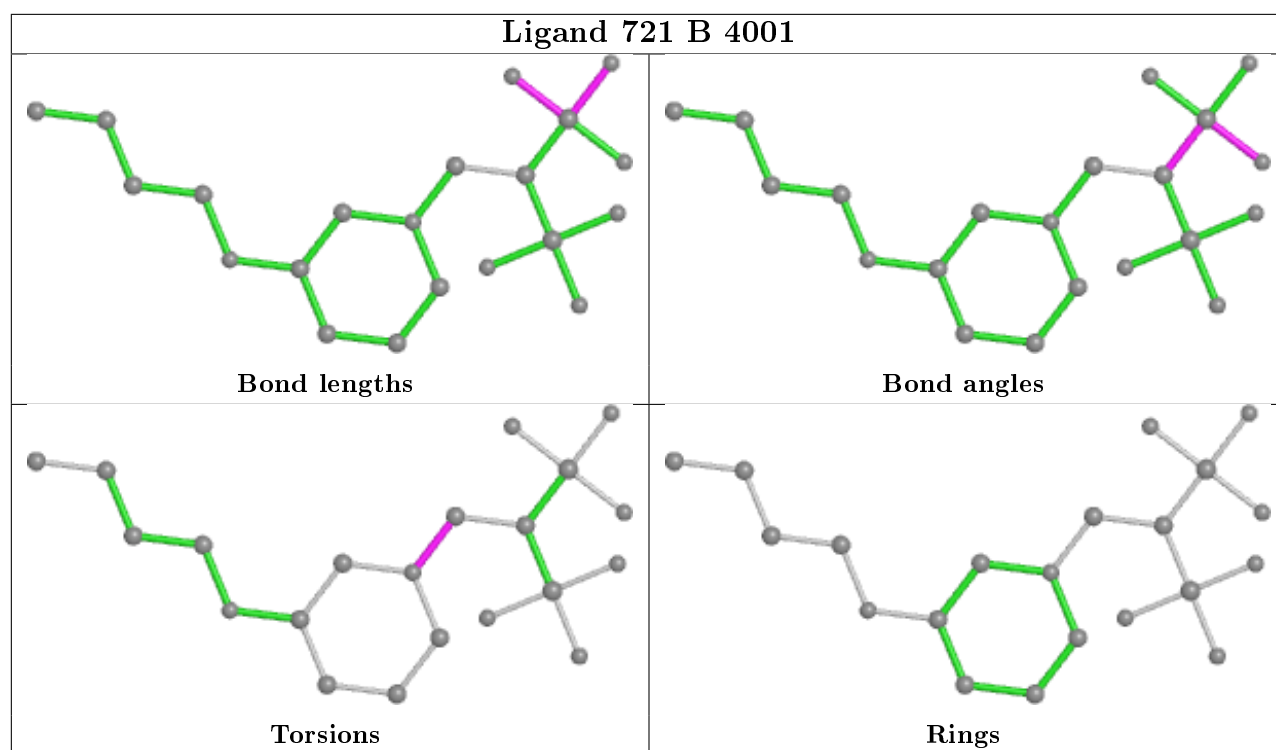
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4001	721	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	358/390 (91%)	1.11	58 (16%)  	25, 42, 58, 68	0
1	B	359/390 (92%)	1.09	56 (15%)  	26, 40, 58, 71	0
All	All	717/780 (91%)	1.10	114 (15%)  	25, 41, 58, 71	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	6.5
1	B	367	LYS	6.3
1	B	73	ASP	5.7
1	A	190	SER	4.6
1	B	308	GLU	4.6
1	B	74	ASP	4.3
1	A	79	LYS	4.2
1	A	267	LEU	4.1
1	B	64	LEU	4.1
1	B	145	MET	4.0
1	A	323	GLN	4.0
1	A	62	LEU	3.8
1	B	270	VAL	3.6
1	A	336	GLN	3.6
1	A	63	SER	3.6
1	B	307	SER	3.5
1	A	57	VAL	3.4
1	B	63	SER	3.4
1	A	4	GLN	3.4
1	A	122	PRO	3.4
1	A	270	VAL	3.4
1	A	55	ILE	3.4
1	A	358	LEU	3.4
1	B	328	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	307	SER	3.3
1	A	15	MET	3.2
1	A	367	LYS	3.2
1	A	145	MET	3.2
1	B	305	GLY	3.1
1	B	317	TYR	3.1
1	A	321	ASP	3.1
1	B	321	ASP	3.1
1	A	5	MET	3.1
1	A	319	GLU	3.0
1	A	360	GLY	3.0
1	B	189	VAL	3.0
1	B	4	GLN	3.0
1	A	192	PRO	3.0
1	A	316	LEU	3.0
1	B	263	PRO	3.0
1	B	320	ALA	3.0
1	A	95	LEU	2.9
1	B	195	THR	2.9
1	A	125	THR	2.8
1	A	74	ASP	2.8
1	B	5	MET	2.7
1	A	76	ALA	2.7
1	B	80	ARG	2.7
1	B	269	LYS	2.7
1	B	2	PRO	2.7
1	A	339	GLU	2.6
1	B	185	LEU	2.6
1	A	47	LYS	2.6
1	B	319	GLU	2.6
1	B	192	PRO	2.6
1	B	197	PHE	2.6
1	A	308	GLU	2.6
1	B	267	LEU	2.6
1	A	150	ASP	2.6
1	B	92	ILE	2.6
1	B	346	LEU	2.5
1	B	366	GLN	2.5
1	B	315	ARG	2.5
1	A	347	CYS	2.5
1	B	276	ASP	2.5
1	A	92	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	362	THR	2.5
1	A	123	ASP	2.5
1	B	274	ILE	2.4
1	B	266	ARG	2.4
1	A	346	LEU	2.4
1	A	54	VAL	2.4
1	B	190	SER	2.4
1	A	133	GLY	2.4
1	A	1	MET	2.4
1	B	62	LEU	2.4
1	B	123	ASP	2.4
1	A	53	THR	2.3
1	A	136	LEU	2.3
1	B	180	PHE	2.3
1	B	122	PRO	2.3
1	B	324	GLY	2.3
1	A	52	LEU	2.3
1	A	161	PHE	2.3
1	B	332	ALA	2.2
1	B	336	GLN	2.2
1	B	354	SER	2.2
1	A	134	LEU	2.2
1	A	335	GLU	2.2
1	B	15	MET	2.2
1	B	302	TYR	2.2
1	A	300	ALA	2.2
1	A	324	GLY	2.2
1	B	312	THR	2.2
1	B	164	VAL	2.2
1	A	305	GLY	2.1
1	A	261	PHE	2.1
1	A	337	VAL	2.1
1	B	310	VAL	2.1
1	A	22	GLU	2.1
1	A	318	GLU	2.1
1	B	141	HIS	2.1
1	B	169	ALA	2.1
1	A	49	ASN	2.1
1	A	298	PHE	2.1
1	B	261	PHE	2.1
1	B	136	LEU	2.1
1	B	222	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	2.0
1	B	273	ASP	2.0
1	A	340	LEU	2.0
1	A	355	VAL	2.0
1	B	161	PHE	2.0
1	A	274	ILE	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](#)

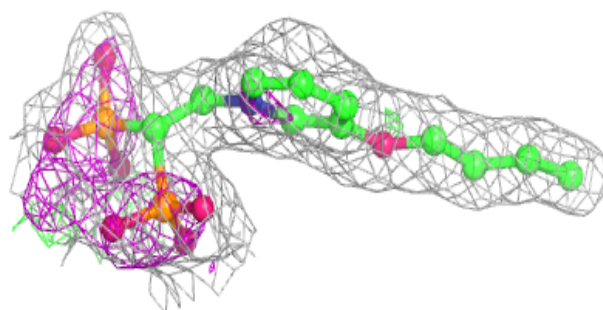
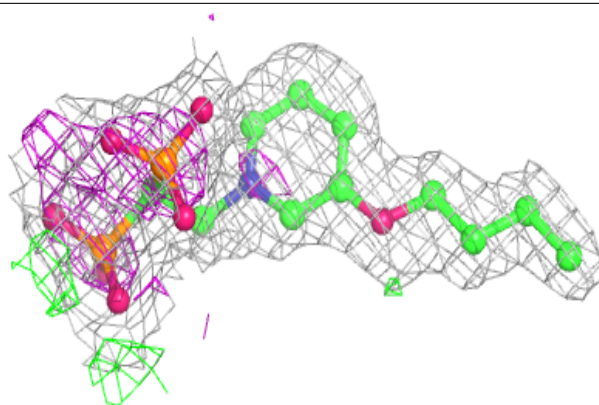
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MG	A	3002	1/1	0.76	0.17	29,29,29,29	0
2	MG	B	4003	1/1	0.86	0.08	34,34,34,34	0
2	MG	A	3003	1/1	0.88	0.09	33,33,33,33	0
3	721	A	3001	21/21	0.94	0.14	24,28,32,35	0
3	721	B	4001	21/21	0.94	0.14	25,32,34,36	0
2	MG	B	4004	1/1	0.95	0.15	29,29,29,29	0
2	MG	B	4002	1/1	0.96	0.19	31,31,31,31	0
2	MG	A	3004	1/1	0.98	0.20	30,30,30,30	0

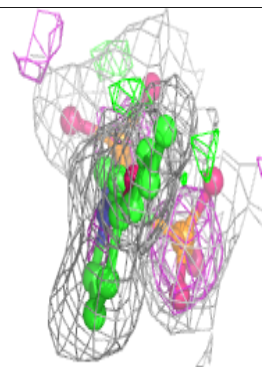
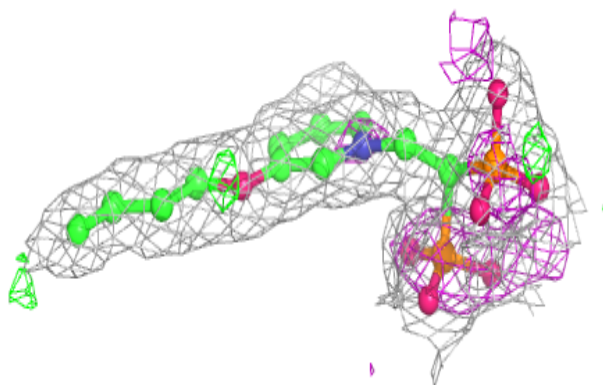
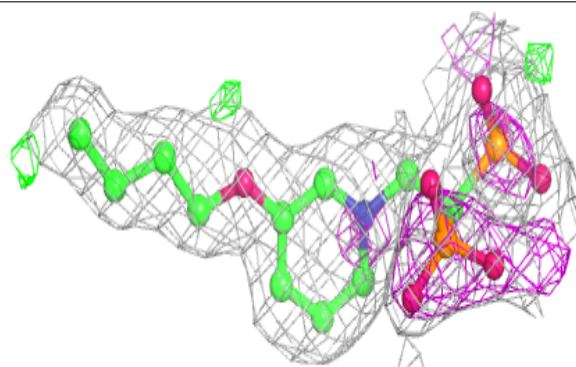
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 721 A 3001:**

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

**Electron density around 721 B 4001:**

$2mF_o-DF_c$  (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.