



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:28 PM BST

PDB ID : 4Q2G  
Title : CRYSTAL STRUCTURE OF AN INTRAMEMBRANE CDP-DAG  
SYNTHETASE CENTRAL FOR PHOSPHOLIPID BIOSYNTHESIS  
(S200C/S223C, inactive mutant)  
Authors : Liu, X.; Yin, Y.; Wu, J.; Liu, Z.  
Deposited on : 2014-04-08  
Resolution : 3.40 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 : 2.13.1  
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) : 2.13.1

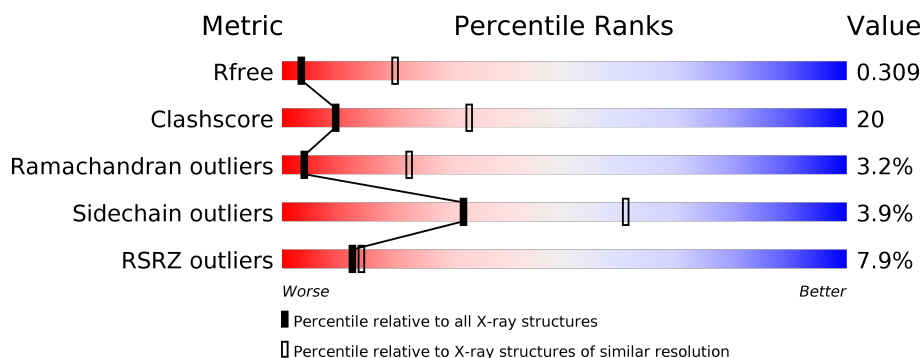
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	290	<div> <div>7%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>• 10%</div> </div> </div>
1	B	290	<div> <div>8%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4236 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 Phosphatidate cytidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2061	1386	316	353	6			
1	B	269	Total	C	N	O	S	0	0	0
			2127	1427	328	366	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9X1B7
A	2	GLY	-	expression tag	UNP Q9X1B7
A	3	SER	-	expression tag	UNP Q9X1B7
A	4	SER	-	expression tag	UNP Q9X1B7
A	5	HIS	-	expression tag	UNP Q9X1B7
A	6	HIS	-	expression tag	UNP Q9X1B7
A	7	HIS	-	expression tag	UNP Q9X1B7
A	8	HIS	-	expression tag	UNP Q9X1B7
A	9	HIS	-	expression tag	UNP Q9X1B7
A	10	HIS	-	expression tag	UNP Q9X1B7
A	11	SER	-	expression tag	UNP Q9X1B7
A	12	SER	-	expression tag	UNP Q9X1B7
A	13	GLY	-	expression tag	UNP Q9X1B7
A	14	LEU	-	expression tag	UNP Q9X1B7
A	15	VAL	-	expression tag	UNP Q9X1B7
A	16	PRO	-	expression tag	UNP Q9X1B7
A	17	ARG	-	expression tag	UNP Q9X1B7
A	18	GLY	-	expression tag	UNP Q9X1B7
A	19	SER	-	expression tag	UNP Q9X1B7
A	20	HIS	-	expression tag	UNP Q9X1B7
A	220	CYS	SER	engineered mutation	UNP Q9X1B7
A	278	CYS	SER	engineered mutation	UNP Q9X1B7
B	1	MET	-	expression tag	UNP Q9X1B7
B	2	GLY	-	expression tag	UNP Q9X1B7
B	3	SER	-	expression tag	UNP Q9X1B7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP Q9X1B7
B	5	HIS	-	expression tag	UNP Q9X1B7
B	6	HIS	-	expression tag	UNP Q9X1B7
B	7	HIS	-	expression tag	UNP Q9X1B7
B	8	HIS	-	expression tag	UNP Q9X1B7
B	9	HIS	-	expression tag	UNP Q9X1B7
B	10	HIS	-	expression tag	UNP Q9X1B7
B	11	SER	-	expression tag	UNP Q9X1B7
B	12	SER	-	expression tag	UNP Q9X1B7
B	13	GLY	-	expression tag	UNP Q9X1B7
B	14	LEU	-	expression tag	UNP Q9X1B7
B	15	VAL	-	expression tag	UNP Q9X1B7
B	16	PRO	-	expression tag	UNP Q9X1B7
B	17	ARG	-	expression tag	UNP Q9X1B7
B	18	GLY	-	expression tag	UNP Q9X1B7
B	19	SER	-	expression tag	UNP Q9X1B7
B	20	HIS	-	expression tag	UNP Q9X1B7
B	220	CYS	SER	engineered mutation	UNP Q9X1B7
B	278	CYS	SER	engineered mutation	UNP Q9X1B7

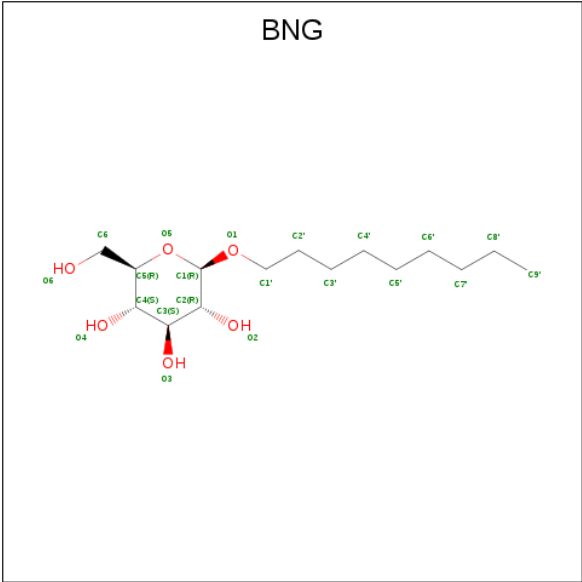
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Hg 2 2	0	0
2	A	2	Total Hg 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).

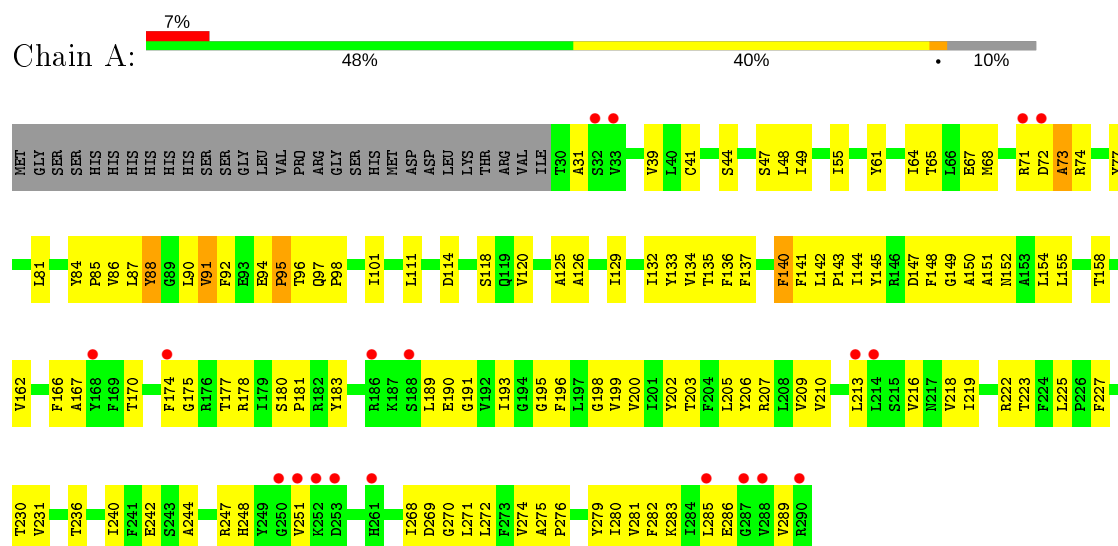


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	B	1	Total	C	O	0	0
			21	15	6		

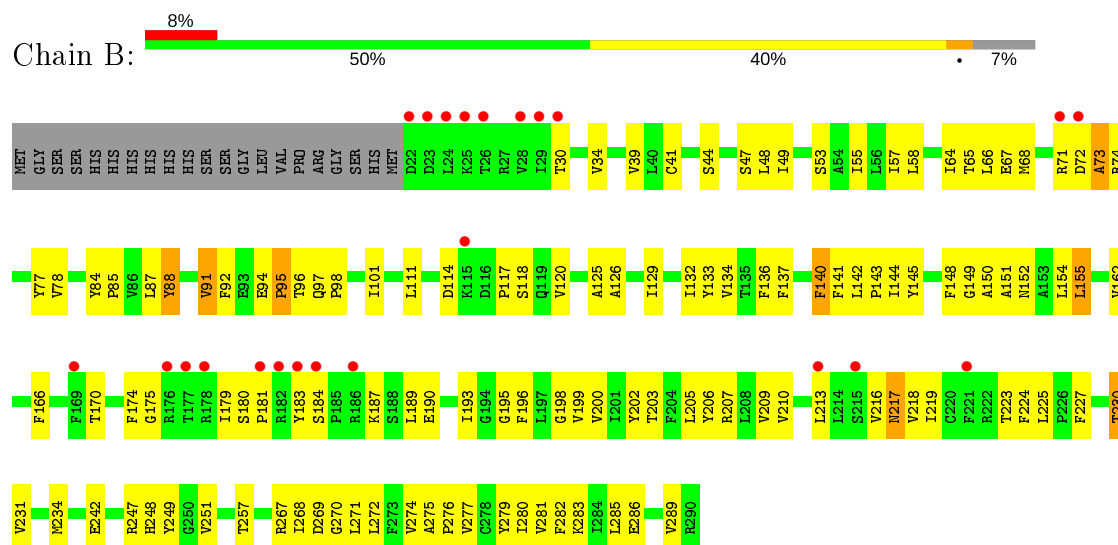
### 3 Residue-property plots

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

#### • Molecule 1: Phosphatidate cytidyltransferase



#### • Molecule 1: Phosphatidate cytidyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.41Å 141.41Å 197.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.10 – 3.40 28.10 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (28.10-3.40) 98.0 (28.10-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.291 , 0.315 0.285 , 0.309	Depositor DCC
$R_{free}$ test set	821 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BNG, HG

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	0.52	0/2115	0.77	0/2877
1	B	0.52	0/2181	0.76	0/2966
All	All	0.52	0/4296	0.77	0/5843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2061	0	2126	84	0
1	B	2127	0	2198	92	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	30	3	0
4	B	21	0	30	3	0
All	All	4236	0	4384	169	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 20.



All (169) 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:B:179:ILE:HD11	1:B:189:LEU:HB2	1.59	0.85
1:A:148:PHE:CE1	1:A:282:PHE:HB3	2.16	0.80
1:B:39:VAL:HG13	1:B:154:LEU:HD11	1.61	0.80
1:B:183:TYR:HB2	1:B:247:ARG:HG3	1.66	0.77
1:A:227:PHE:O	1:A:231:VAL:HG23	1.85	0.76
1:A:67:GLU:HG3	1:A:126:ALA:HB2	1.68	0.75
1:A:39:VAL:HG13	1:A:154:LEU:HD11	1.68	0.75
1:B:227:PHE:O	1:B:231:VAL:HG23	1.87	0.74
1:B:67:GLU:HG3	1:B:126:ALA:HB2	1.70	0.73
1:B:162:VAL:HG21	1:B:202:TYR:CD1	2.22	0.73
1:B:223:THR:HG22	1:B:285:LEU:HB3	1.71	0.72
1:A:162:VAL:HG21	1:A:202:TYR:CD1	2.25	0.71
1:A:125:ALA:HB1	1:B:125:ALA:HB1	1.71	0.71
1:B:133:TYR:O	1:B:137:PHE:HB2	1.91	0.70
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.73	0.70
1:A:68:MET:SD	1:A:73:ALA:HB1	2.32	0.70
1:A:170:THR:O	1:A:174:PHE:HB2	1.93	0.69
1:A:223:THR:HG22	1:A:285:LEU:HB3	1.74	0.68
1:A:41:CYS:SG	2:A:302:HG:HG	2.12	0.68
1:A:55:ILE:HD13	4:A:304:BNG:H5'2	1.76	0.67
1:B:41:CYS:SG	2:B:302:HG:HG	2.13	0.67
1:B:275:ALA:HB3	1:B:276:PRO:HD3	1.76	0.67
1:B:88:TYR:O	1:B:88:TYR:HD1	1.77	0.66
1:A:97:GLN:HE21	1:B:280:ILE:HA	1.61	0.66
1:B:148:PHE:CE1	1:B:282:PHE:HB3	2.31	0.66
1:B:189:LEU:O	1:B:193:ILE:HG13	1.96	0.66
1:B:68:MET:SD	1:B:73:ALA:HB1	2.37	0.65
1:A:189:LEU:O	1:A:193:ILE:HG13	1.97	0.65
1:A:88:TYR:HD1	1:A:88:TYR:O	1.78	0.65
1:A:195:GLY:O	1:A:199:VAL:HG23	1.97	0.65
1:B:162:VAL:HG21	1:B:202:TYR:CE1	2.32	0.64
1:A:141:PHE:HZ	1:A:271:LEU:HD11	1.62	0.64
1:A:279:TYR:OH	1:A:283:LYS:HE2	1.98	0.63
1:A:55:ILE:HG21	1:A:268:ILE:HD11	1.80	0.63
1:B:279:TYR:OH	1:B:283:LYS:HE2	1.99	0.63
1:A:133:TYR:O	1:A:137:PHE:HB2	1.99	0.62
1:B:67:GLU:HG2	1:B:249:TYR:OH	1.99	0.62
1:B:170:THR:O	1:B:174:PHE:HB2	2.00	0.61
1:B:230:THR:HG21	1:B:281:VAL:HG21	1.83	0.60
1:A:44:SER:HB2	1:A:47:SER:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLY:O	1:B:199:VAL:HG23	2.01	0.60
1:B:223:THR:HG22	1:B:285:LEU:CB	2.32	0.60
1:A:223:THR:HG22	1:A:285:LEU:CB	2.32	0.60
1:A:270:GLY:O	1:A:274:VAL:HG23	2.02	0.60
1:B:270:GLY:O	1:B:274:VAL:HG23	2.03	0.59
1:A:230:THR:HG21	1:A:281:VAL:HG21	1.84	0.59
1:B:140:PHE:CD2	1:B:276:PRO:HA	2.38	0.57
1:B:140:PHE:O	1:B:144:ILE:HG13	2.05	0.57
1:A:271:LEU:HD21	4:A:304:BNG:H7'1	1.85	0.57
1:A:140:PHE:O	1:A:144:ILE:HG13	2.05	0.57
1:A:140:PHE:CD2	1:A:276:PRO:HA	2.39	0.57
1:B:44:SER:HB2	1:B:47:SER:H	1.70	0.57
1:B:180:SER:HB3	1:B:187:LYS:HB2	1.86	0.56
1:A:248:HIS:HB2	1:B:118:SER:HA	1.87	0.55
1:A:88:TYR:C	1:A:88:TYR:CD1	2.79	0.55
1:B:88:TYR:CD1	1:B:88:TYR:C	2.80	0.55
1:B:267:ARG:HH11	4:B:304:BNG:H1'1	1.73	0.54
1:A:65:THR:OG1	1:A:74:ARG:HD2	2.08	0.53
1:B:219:ILE:HG23	1:B:223:THR:OG1	2.08	0.53
1:B:175:GLY:HA3	1:B:190:GLU:OE1	2.08	0.53
1:A:55:ILE:CG2	1:A:268:ILE:HD11	2.38	0.53
1:A:167:ALA:HA	1:A:191:GLY:O	2.09	0.53
1:B:65:THR:OG1	1:B:74:ARG:HD2	2.09	0.53
1:A:166:PHE:CD2	1:A:198:GLY:HA3	2.44	0.53
1:A:242:GLU:O	1:A:242:GLU:HG2	2.09	0.52
1:B:39:VAL:HG22	1:B:154:LEU:HD21	1.91	0.52
1:B:141:PHE:HZ	1:B:271:LEU:HD11	1.74	0.52
1:B:55:ILE:CG2	1:B:268:ILE:HD11	2.40	0.52
1:A:92:PHE:C	1:A:94:GLU:H	2.13	0.51
1:A:118:SER:HA	1:B:248:HIS:HB2	1.93	0.51
1:B:92:PHE:C	1:B:94:GLU:H	2.13	0.51
1:A:196:PHE:O	1:A:200:VAL:HG23	2.11	0.51
1:B:74:ARG:O	1:B:78:VAL:HG23	2.11	0.51
1:B:268:ILE:O	1:B:271:LEU:HB3	2.11	0.50
1:A:280:ILE:HA	1:B:97:GLN:HE21	1.75	0.50
1:A:114:ASP:HB2	1:A:120:VAL:HG22	1.93	0.50
1:B:196:PHE:O	1:B:200:VAL:HG23	2.12	0.50
1:A:73:ALA:O	1:A:77:TYR:HD2	1.94	0.50
1:A:141:PHE:CZ	1:A:271:LEU:HD11	2.44	0.49
1:B:268:ILE:HG22	1:B:272:LEU:HG	1.94	0.49
1:A:39:VAL:HG22	1:A:154:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:O	1:B:34:VAL:HG23	2.13	0.49
1:A:219:ILE:HG23	1:A:223:THR:OG1	2.12	0.49
1:B:242:GLU:HG2	1:B:242:GLU:O	2.12	0.48
1:B:223:THR:HG21	1:B:286:GLU:HG3	1.95	0.48
1:A:141:PHE:CE2	4:A:304:BNG:H8'2	2.49	0.48
1:A:210:VAL:O	1:A:216:VAL:HB	2.12	0.48
1:B:73:ALA:O	1:B:77:TYR:HD2	1.96	0.48
1:A:152:ASN:O	1:A:155:LEU:HB3	2.13	0.48
1:B:67:GLU:HG2	1:B:249:TYR:CE2	2.49	0.48
1:A:84:TYR:HB3	1:A:85:PRO:HD3	1.96	0.48
1:A:87:LEU:HD23	1:A:91:VAL:HG21	1.95	0.47
1:A:272:LEU:O	1:A:276:PRO:HD2	2.14	0.47
1:A:67:GLU:HG3	1:A:126:ALA:CB	2.41	0.47
1:B:55:ILE:HD13	4:B:304:BNG:H8'2	1.95	0.47
1:A:175:GLY:HA3	1:A:190:GLU:OE1	2.15	0.47
1:A:95:PRO:HG2	1:A:96:THR:H	1.79	0.47
1:A:111:LEU:HD23	1:A:120:VAL:HG11	1.98	0.46
1:B:267:ARG:HD3	4:B:304:BNG:H1'1	1.96	0.46
1:A:152:ASN:OD1	1:A:219:ILE:HG13	2.15	0.46
1:A:205:LEU:O	1:A:209:VAL:HG23	2.16	0.46
1:B:87:LEU:HD23	1:B:91:VAL:HG21	1.98	0.46
1:B:111:LEU:HD23	1:B:120:VAL:HG11	1.97	0.46
1:A:97:GLN:NE2	1:B:280:ILE:HA	2.29	0.46
1:B:114:ASP:HB2	1:B:120:VAL:HG22	1.97	0.46
1:B:166:PHE:CD2	1:B:198:GLY:HA3	2.51	0.46
1:A:132:ILE:O	1:A:136:PHE:HB3	2.16	0.46
1:B:66:LEU:HB3	1:B:249:TYR:CG	2.51	0.46
1:A:223:THR:HG21	1:A:286:GLU:HG3	1.98	0.46
1:B:88:TYR:HD1	1:B:88:TYR:C	2.19	0.45
1:B:210:VAL:O	1:B:216:VAL:HB	2.16	0.45
1:B:95:PRO:HG2	1:B:96:THR:H	1.81	0.45
1:A:152:ASN:HA	1:A:155:LEU:HB3	1.98	0.45
1:B:272:LEU:O	1:B:276:PRO:HD2	2.16	0.45
1:B:282:PHE:O	1:B:286:GLU:N	2.48	0.45
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.68	0.45
1:B:64:ILE:HD13	1:B:77:TYR:HB2	1.99	0.45
1:B:181:PRO:HD2	1:B:184:SER:HB3	1.98	0.45
1:B:234:MET:SD	1:B:277:VAL:HG21	2.57	0.45
1:B:217:ASN:HD21	1:B:289:VAL:HB	1.82	0.44
1:A:268:ILE:O	1:A:271:LEU:HB3	2.18	0.44
1:A:147:ASP:HA	1:A:289:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:TYR:O	1:B:88:TYR:CD1	2.64	0.44
1:B:98:PRO:HA	1:B:101:ILE:HG12	2.00	0.43
1:B:149:GLY:O	1:B:151:ALA:N	2.51	0.43
1:B:67:GLU:HG3	1:B:126:ALA:CB	2.44	0.43
1:A:282:PHE:O	1:A:286:GLU:N	2.51	0.43
1:B:125:ALA:O	1:B:129:ILE:HG13	2.18	0.43
1:B:58:LEU:HD22	1:B:257:THR:HG21	2.00	0.43
1:A:61:TYR:CD2	1:A:61:TYR:C	2.91	0.43
1:A:72:ASP:O	1:A:73:ALA:C	2.56	0.43
1:A:49:ILE:HG12	1:A:142:LEU:HD21	2.00	0.43
1:A:206:TYR:CE2	1:A:210:VAL:HG21	2.54	0.43
1:A:64:ILE:HD13	1:A:77:TYR:HB2	2.01	0.43
1:A:48:LEU:HD22	1:A:145:TYR:CD1	2.54	0.42
1:A:88:TYR:HD1	1:A:88:TYR:C	2.19	0.42
1:A:154:LEU:O	1:A:158:THR:HG23	2.19	0.42
1:B:205:LEU:O	1:B:209:VAL:HG23	2.19	0.42
1:B:148:PHE:CZ	1:B:282:PHE:HB3	2.54	0.42
1:B:72:ASP:O	1:B:73:ALA:C	2.58	0.42
1:A:98:PRO:HA	1:A:101:ILE:HG12	2.01	0.42
1:B:49:ILE:HG12	1:B:142:LEU:HD21	2.01	0.42
1:A:202:TYR:O	1:A:206:TYR:HB2	2.19	0.42
1:A:86:VAL:HG13	1:A:90:LEU:HD12	2.02	0.42
1:A:125:ALA:O	1:A:129:ILE:HG13	2.20	0.42
1:A:149:GLY:O	1:A:151:ALA:N	2.53	0.42
1:B:132:ILE:O	1:B:136:PHE:HB3	2.20	0.42
1:B:162:VAL:HG11	1:B:202:TYR:HB2	2.01	0.42
1:B:84:TYR:HB3	1:B:85:PRO:HD3	2.02	0.42
1:A:140:PHE:C	1:A:143:PRO:HD2	2.40	0.42
1:B:289:VAL:HG23	1:B:289:VAL:O	2.20	0.42
1:B:152:ASN:HA	1:B:155:LEU:HB3	2.02	0.41
1:B:203:THR:HB	1:B:224:PHE:CE1	2.55	0.41
1:A:81:LEU:HD22	1:A:135:THR:OG1	2.20	0.41
1:B:53:SER:O	1:B:57:ILE:HG13	2.20	0.41
1:A:148:PHE:CZ	1:A:282:PHE:HB3	2.54	0.41
1:A:183:TYR:CE1	1:A:244:ALA:HB2	2.55	0.41
1:B:202:TYR:O	1:B:206:TYR:HB2	2.20	0.41
1:A:222:ARG:HD3	1:A:222:ARG:HA	1.92	0.41
1:B:67:GLU:HG2	1:B:249:TYR:CZ	2.55	0.41
1:A:189:LEU:HG	1:A:193:ILE:HD11	2.02	0.41
1:A:247:ARG:HB2	1:B:117:PRO:HB2	2.03	0.41
1:B:140:PHE:C	1:B:143:PRO:HD2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HG	1:B:193:ILE:HD11	2.02	0.41
1:B:48:LEU:HD22	1:B:145:TYR:CD1	2.56	0.41
1:B:219:ILE:HA	1:B:286:GLU:OE2	2.22	0.40
1:A:236:THR:O	1:A:240:ILE:HG13	2.21	0.40
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.83	0.40
1:A:180:SER:HA	1:A:181:PRO:HD3	1.89	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	259/290 (89%)	221 (85%)	29 (11%)	9 (4%)	3	21
1	B	267/290 (92%)	230 (86%)	29 (11%)	8 (3%)	4	23
All	All	526/580 (91%)	451 (86%)	58 (11%)	17 (3%)	4	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	213	LEU
1	A	269	ASP
1	B	71	ARG
1	B	213	LEU
1	A	95	PRO
1	B	150	ALA
1	A	31	ALA
1	B	73	ALA
1	B	95	PRO
1	B	269	ASP
1	A	73	ALA

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Mol	Chain	Res	Type
1	A	150	ALA
1	A	91	VAL
1	A	134	VAL
1	B	91	VAL
1	B	134	VAL

### 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	224/250 (90%)	215 (96%)	9 (4%)	31	60
1	B	232/250 (93%)	223 (96%)	9 (4%)	32	61
All	All	456/500 (91%)	438 (96%)	18 (4%)	32	61

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	TYR
1	A	140	PHE
1	A	177	THR
1	A	178	ARG
1	A	203	THR
1	A	207	ARG
1	A	218	VAL
1	A	225	LEU
1	A	251	VAL
1	B	88	TYR
1	B	140	PHE
1	B	155	LEU
1	B	207	ARG
1	B	217	ASN
1	B	218	VAL
1	B	225	LEU
1	B	230	THR
1	B	251	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	248	HIS
1	B	97	GLN
1	B	217	ASN

### 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 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	$\# Z  > 2$
4	BNG	A	304	-	21,21,21	0.57	0	26,26,26	0.81	1 (3%)
4	BNG	B	304	-	21,21,21	0.58	0	26,26,26	1.37	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BNG	A	304	-	-	3/12/32/32	0/1/1/1
4	BNG	B	304	-	-	5/12/32/32	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	BNG	C3-C4-C5	4.90	118.97	110.24
4	B	304	BNG	C4-C3-C2	3.05	116.15	110.82
4	B	304	BNG	C1'-O1-C1	2.53	118.03	113.84
4	A	304	BNG	C1'-O1-C1	2.31	117.67	113.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	304	BNG	O5-C1-O1-C1'
4	B	304	BNG	C4-C5-C6-O6
4	B	304	BNG	O5-C5-C6-O6
4	A	304	BNG	O1-C1'-C2'-C3'
4	B	304	BNG	C2-C1-O1-C1'
4	B	304	BNG	C5'-C6'-C7'-C8'
4	A	304	BNG	C3'-C4'-C5'-C6'
4	A	304	BNG	C6'-C7'-C8'-C9'

There are no ring outliers.

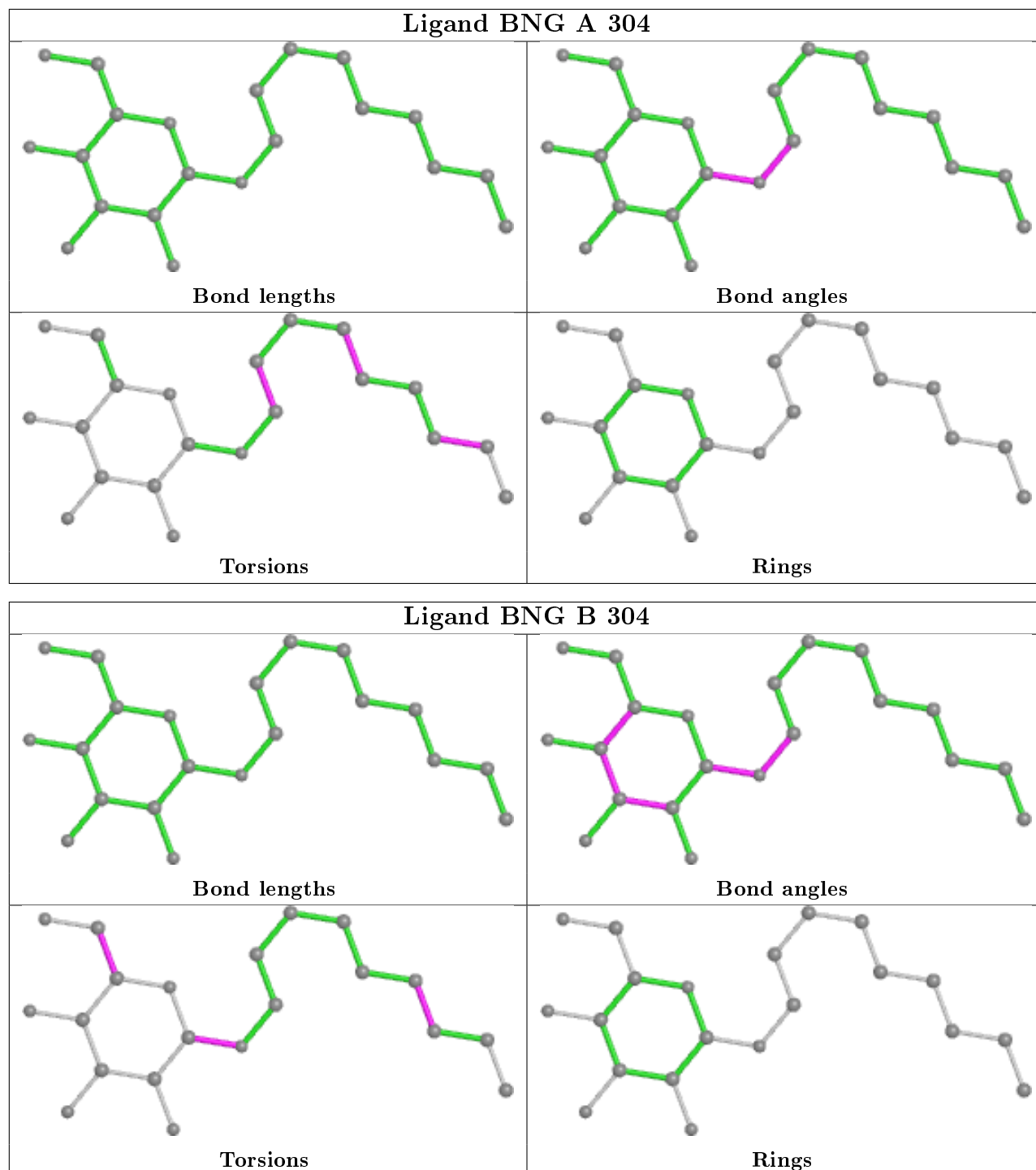
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	BNG	3	0
4	B	304	BNG	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	261/290 (90%)	-0.00	19 (7%) 15 17	67, 110, 166, 187	0
1	B	269/290 (92%)	-0.08	23 (8%) 10 12	66, 111, 176, 210	0
All	All	530/580 (91%)	-0.04	42 (7%) 12 14	66, 111, 172, 210	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	LEU	6.0
1	A	287	GLY	4.9
1	A	213	LEU	4.9
1	B	23	ASP	4.7
1	A	174	PHE	4.6
1	B	22	ASP	4.3
1	A	32	SER	4.2
1	B	182	ARG	4.0
1	B	30	THR	4.0
1	B	215	SER	4.0
1	B	186	ARG	3.8
1	B	176	ARG	3.8
1	B	213	LEU	3.5
1	A	252	LYS	3.5
1	A	168	TYR	3.4
1	A	33	VAL	3.3
1	A	251	VAL	3.1
1	A	261	HIS	3.1
1	B	115	LYS	3.1
1	A	290	ARG	3.1
1	B	178	ARG	3.0
1	A	250	GLY	2.9
1	B	184	SER	2.8
1	B	169	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	28	VAL	2.7
1	B	25	LYS	2.7
1	B	177	THR	2.7
1	A	253	ASP	2.7
1	B	181	PRO	2.7
1	B	29	ILE	2.7
1	B	183	TYR	2.6
1	A	285	LEU	2.5
1	A	214	LEU	2.4
1	A	188	SER	2.3
1	B	26	THR	2.3
1	B	72	ASP	2.2
1	A	71	ARG	2.2
1	A	186	ARG	2.1
1	B	221	PHE	2.1
1	A	288	VAL	2.1
1	A	72	ASP	2.1
1	B	71	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.

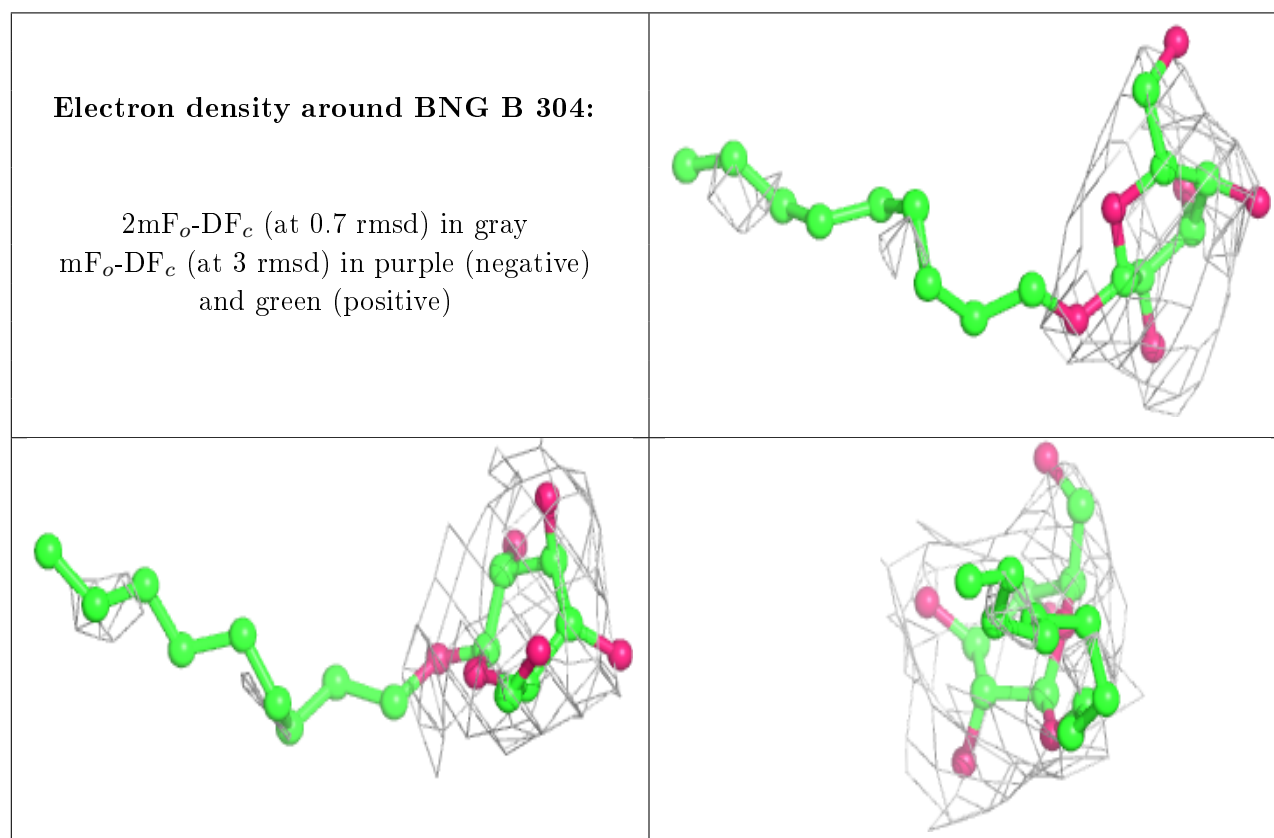
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HG	B	301	1/1	0.55	0.28	260,260,260,260	0
2	HG	A	301	1/1	0.78	0.11	232,232,232,232	0
3	MG	B	303	1/1	0.87	0.38	119,119,119,119	0
4	BNG	B	304	21/21	0.92	0.26	112,125,127,128	0
4	BNG	A	304	21/21	0.92	0.26	97,114,118,119	0

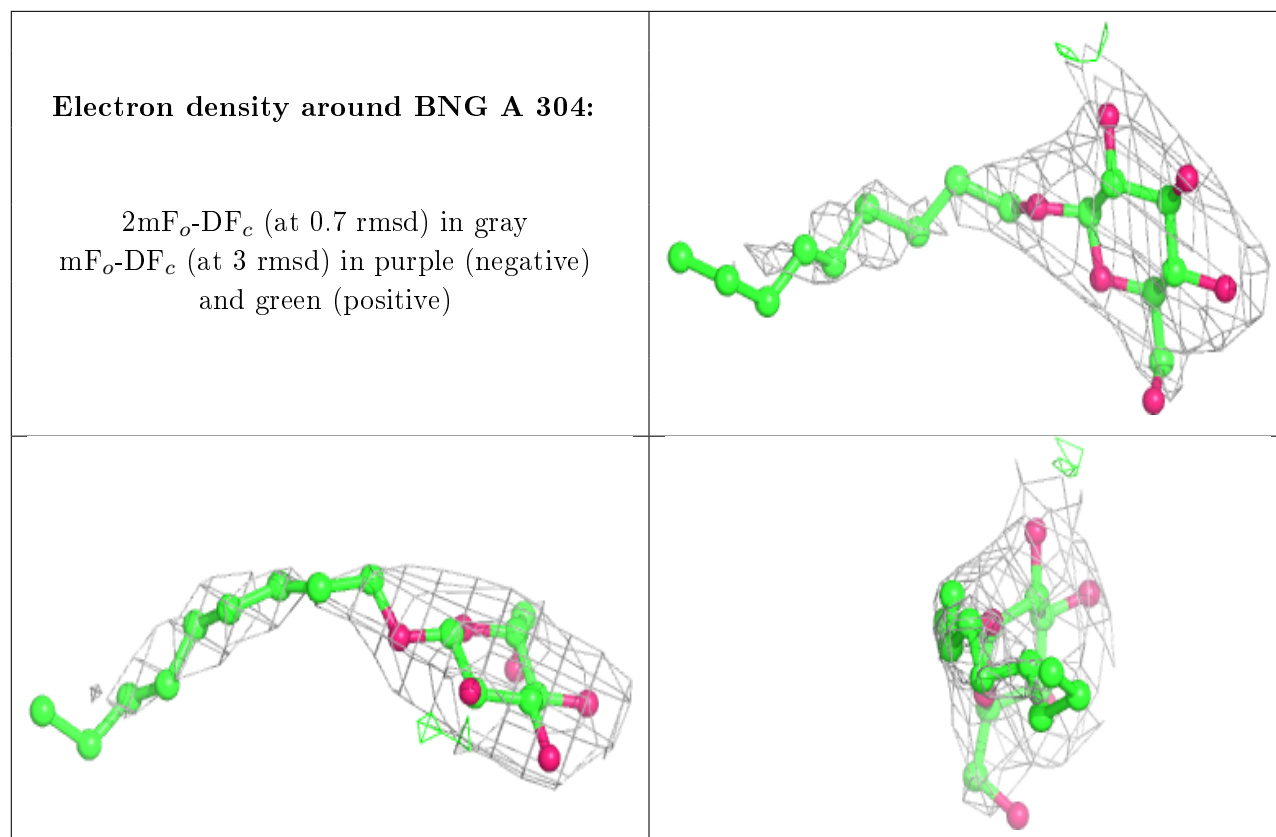
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	303	1/1	0.94	0.28	108,108,108,108	0
2	HG	A	302	1/1	0.97	0.03	172,172,172,172	0
2	HG	B	302	1/1	0.99	0.02	162,162,162,162	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.