



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:52 AM UTC

PDB ID : 2E92 / pdb_00002e92
Title : S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium and BPH-261
Authors : Guo, R.T.; Ko, T.P.; Cao, R.; Jeng, W.Y.; Chen, C.K.-M.; Chang, T.H.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.
Deposited on : 2007-01-24
Resolution : 2.31 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

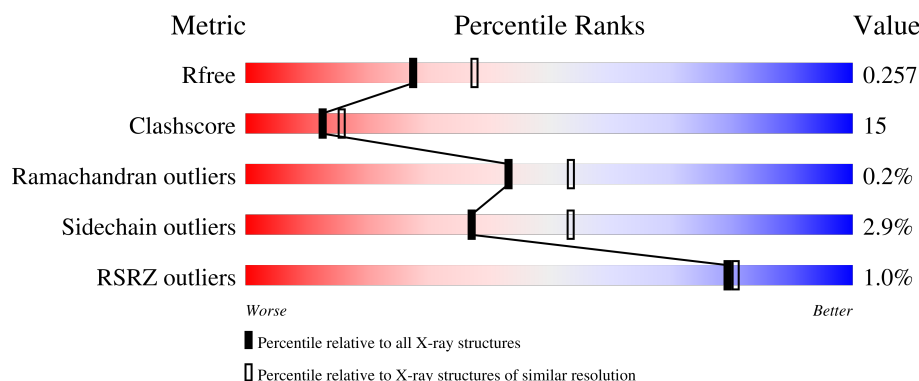
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	340	
1	B	340	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	M0N	A	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5111 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 Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2373	1524	400	439	10			
1	B	290	Total	C	N	O	S	0	0	0
			2368	1523	400	435	10			

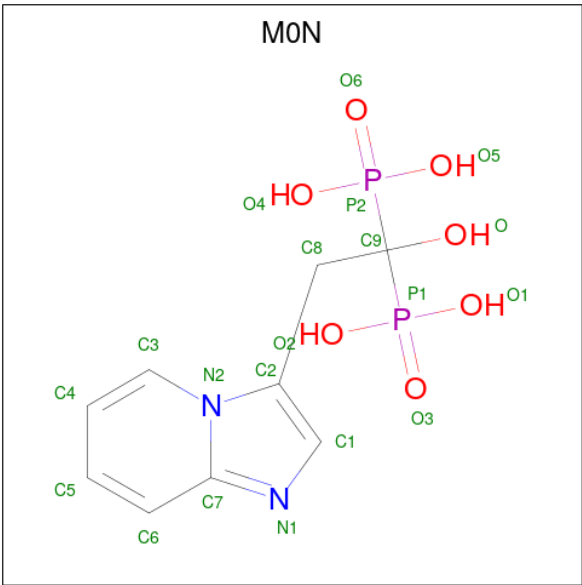
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q12051
A	2	THR	-	cloning artifact	UNP Q12051
A	3	LYS	-	cloning artifact	UNP Q12051
A	4	ASN	-	cloning artifact	UNP Q12051
A	5	LYS	-	cloning artifact	UNP Q12051
B	1	MET	-	cloning artifact	UNP Q12051
B	2	THR	-	cloning artifact	UNP Q12051
B	3	LYS	-	cloning artifact	UNP Q12051
B	4	ASN	-	cloning artifact	UNP Q12051
B	5	LYS	-	cloning artifact	UNP Q12051

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is (1-HYDROXY-2-IMIDAZO[1,2-A]PYRIDIN-3-YLETHANE-1,1-DIYL)BIS(P HOSPHONIC ACID) (CCD ID: M0N) (formula: C₉H₁₂N₂O₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	7	2		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	176	Total	O	0	0
			176	176		

- Molecule 1: Geranylgeranyl pyrophosphate synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.87Å 116.05Å 127.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.31 30.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.00-2.31) 91.3 (30.00-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.257 0.199 , 0.257	Depositor DCC
R_{free} test set	1397 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, M0N

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	0.90	3/2413 (0.1%)	1.14	14/3265 (0.4%)
1	B	0.85	0/2408	1.09	13/3257 (0.4%)
All	All	0.87	3/4821 (0.1%)	1.12	27/6522 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	VAL	CA-CB	9.22	1.58	1.54
1	A	166	MET	SD-CE	-5.71	1.65	1.79
1	A	161	ILE	CA-CB	5.59	1.59	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	N-CA-C	-8.09	102.54	111.36
1	A	82	ILE	N-CA-C	-7.48	103.50	110.53
1	A	17	ASP	CA-C-N	-7.18	112.58	119.76
1	A	17	ASP	C-N-CA	-7.18	112.58	119.76
1	B	161	ILE	CA-C-N	-7.00	113.10	120.03
1	B	161	ILE	C-N-CA	-7.00	113.10	120.03
1	B	44	ARG	N-CA-C	-6.91	103.68	111.14
1	A	174	LYS	N-CA-C	6.77	119.24	111.11
1	A	161	ILE	N-CA-C	-6.61	100.53	107.60
1	B	285	PHE	N-CA-C	6.08	119.17	111.69
1	B	54	VAL	N-CA-C	-6.04	107.97	113.71
1	A	95	SER	N-CA-C	5.91	118.49	111.33
1	A	282	ILE	N-CA-C	-5.61	105.26	110.53
1	A	121	GLN	N-CA-C	-5.52	105.76	112.88
1	B	190	SER	N-CA-C	5.51	117.41	109.48
1	B	270	THR	N-CA-C	5.48	119.03	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	GLU	N-CA-C	5.45	120.90	113.16
1	A	53	ARG	N-CA-C	-5.41	106.76	113.19
1	B	147	GLN	N-CA-C	-5.32	105.48	111.28
1	B	10	ILE	N-CA-C	-5.29	105.22	110.62
1	B	121	GLN	N-CA-C	-5.29	106.60	113.16
1	A	238	LYS	N-CA-C	5.19	117.82	110.50
1	A	44	ARG	N-CA-C	-5.12	105.82	111.71
1	A	154	ARG	N-CA-C	5.12	116.55	111.07
1	B	170	MET	N-CA-C	-5.05	105.68	111.14
1	B	65	VAL	N-CA-C	-5.02	105.60	110.42
1	A	101	VAL	CB-CA-C	-5.01	108.94	113.70

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	2373	0	2421	79	0
1	B	2368	0	2425	72	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	20	0	8	8	0
3	B	20	0	8	5	0
4	A	150	0	0	3	0
4	B	176	0	0	3	0
All	All	5111	0	4862	147	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 15.

All (147) 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:143:LEU:HD11	3:B:902:M0N:H5	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:H	1:A:166:MET:HE3	0.93	1.04
1:A:163:THR:N	1:A:166:MET:HE3	1.78	0.97
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.01	0.97
1:A:163:THR:H	1:A:166:MET:CE	1.82	0.93
1:A:139:GLU:HB2	1:A:181:LEU:HD12	1.50	0.92
1:B:55:MET:HE2	1:B:187:GLU:HA	1.49	0.92
1:A:258:GLN:HE21	1:A:258:GLN:H	0.92	0.92
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.51	0.90
1:A:180:ARG:HH11	1:A:204:ASN:ND2	1.69	0.88
1:A:52:ASN:HD21	1:A:57:LEU:H	1.21	0.86
1:A:258:GLN:HE21	1:A:258:GLN:N	1.73	0.86
1:B:52:ASN:HD21	1:B:57:LEU:H	1.23	0.86
1:A:123:THR:HG22	1:A:125:LYS:H	1.40	0.84
1:A:143:LEU:HD11	3:A:901:M0N:H5	1.59	0.83
1:A:76:SER:HB3	3:A:901:M0N:H4	1.66	0.78
1:B:157:LEU:HD12	1:B:158:PRO:HA	1.64	0.78
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.31	0.77
1:A:258:GLN:H	1:A:258:GLN:NE2	1.78	0.73
1:A:143:LEU:HD11	3:A:901:M0N:C5	2.20	0.71
1:B:143:LEU:HD11	3:B:902:M0N:C5	2.13	0.71
1:A:94:THR:HG21	1:A:96:HIS:CE1	2.27	0.70
1:A:148:GLY:C	1:B:28:ILE:HD11	2.17	0.69
1:B:55:MET:CE	1:B:187:GLU:HA	2.23	0.68
3:A:901:M0N:O2	4:A:723:HOH:O	2.12	0.68
1:B:258:GLN:HG3	1:B:286:ASP:OD2	1.93	0.68
1:A:45:LEU:O	1:A:49:VAL:HG23	1.93	0.68
1:B:143:LEU:CD1	3:B:902:M0N:H5	2.15	0.68
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.93	0.67
1:B:258:GLN:OE1	1:B:282:ILE:HD13	1.94	0.66
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.78	0.66
3:A:901:M0N:O6	4:A:723:HOH:O	2.14	0.66
1:A:52:ASN:ND2	1:A:57:LEU:H	1.94	0.65
1:B:52:ASN:ND2	1:B:57:LEU:H	1.96	0.63
1:A:116:MET:HE2	1:B:116:MET:SD	2.39	0.63
1:A:76:SER:HB3	3:A:901:M0N:C4	2.29	0.62
1:B:126:GLU:OE2	1:B:126:GLU:HA	1.99	0.62
1:A:123:THR:HG22	1:A:124:THR:H	1.65	0.62
1:B:55:MET:O	1:B:191:PRO:HD2	1.99	0.61
1:B:52:ASN:HD22	1:B:55:MET:HB2	1.65	0.61
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.82	0.60
1:A:123:THR:CG2	1:A:128:LEU:HD23	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.69	0.58
1:A:94:THR:CG2	1:A:96:HIS:CE1	2.87	0.58
1:B:120:SER:HB3	1:B:129:TYR:CE1	2.38	0.57
1:B:42:ASN:N	4:B:691:HOH:O	2.38	0.57
1:A:283:LEU:HB3	1:A:289:SER:HB2	1.86	0.57
1:A:163:THR:HG23	1:A:166:MET:CE	2.37	0.55
1:A:180:ARG:NH1	1:A:204:ASN:ND2	2.49	0.55
1:A:52:ASN:C	1:A:54:VAL:H	2.12	0.55
1:A:123:THR:HG22	1:A:124:THR:N	2.22	0.55
1:B:215:ASP:HB3	1:B:240:SER:HB2	1.88	0.54
1:B:55:MET:HE3	1:B:190:SER:HB2	1.90	0.53
1:B:119:VAL:HG11	1:B:133:ILE:HD13	1.90	0.53
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.89	0.53
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.74	0.53
1:A:145:ARG:HB3	1:B:20:TRP:CZ3	2.44	0.53
1:A:140:LEU:O	1:A:144:HIS:HD2	1.91	0.53
1:B:75:SER:OG	1:B:111:MET:HB2	2.09	0.52
1:B:183:LEU:HD11	1:B:199:LEU:HB2	1.90	0.52
1:A:47:LEU:O	1:A:51:ILE:HG13	2.10	0.52
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.58	0.51
1:B:167:TYR:C	1:B:167:TYR:CD2	2.89	0.51
1:B:5:LYS:O	1:B:9:LYS:HG3	2.10	0.51
1:B:52:ASN:C	1:B:54:VAL:H	2.18	0.51
1:A:299:GLN:HG2	4:A:569:HOH:O	2.11	0.51
1:B:46:ASN:O	1:B:50:GLN:HG2	2.11	0.51
1:B:230:PHE:O	1:B:276:LYS:NZ	2.42	0.51
1:A:180:ARG:O	1:A:184:ARG:HG3	2.10	0.50
1:B:260:ASN:O	1:B:264:ARG:HG3	2.11	0.50
1:A:145:ARG:HD3	1:B:20:TRP:CD2	2.47	0.50
1:A:5:LYS:O	1:A:9:LYS:HG3	2.12	0.50
1:B:47:LEU:O	1:B:51:ILE:HG13	2.12	0.49
1:A:132:LEU:HD11	1:A:189:LEU:HD21	1.93	0.49
1:A:281:GLN:NE2	1:A:281:GLN:HA	2.27	0.49
1:A:52:ASN:C	1:A:54:VAL:N	2.70	0.49
1:A:126:GLU:N	1:A:127:PRO:CD	2.75	0.49
1:B:128:LEU:O	1:B:132:LEU:HG	2.11	0.49
1:B:62:LEU:HD11	1:B:186:MET:HE3	1.93	0.49
1:B:32:TYR:CD1	1:B:111:MET:HG3	2.48	0.48
1:B:233:ASP:CG	1:B:238:LYS:HD3	2.39	0.48
1:A:234:ILE:HG12	1:A:279:LEU:HD23	1.94	0.48
1:A:255:GLN:HB3	1:A:258:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:902:M0N:O	3:B:902:M0N:H1	2.14	0.48
1:A:143:LEU:HD11	3:A:901:M0N:C6	2.44	0.47
1:B:147:GLN:HE21	1:B:174:LYS:HG3	1.78	0.47
1:B:34:HIS:HE1	1:B:93:THR:O	1.97	0.47
1:B:55:MET:HE3	1:B:190:SER:CB	2.45	0.47
1:B:87:PRO:HA	1:B:97:LEU:HD11	1.96	0.47
1:B:116:MET:O	1:B:119:VAL:HB	2.14	0.47
1:B:132:LEU:HD11	1:B:189:LEU:HD21	1.96	0.47
1:A:139:GLU:HA	1:A:139:GLU:OE2	2.15	0.47
1:A:284:GLU:HB2	1:A:290:LEU:HD12	1.97	0.46
1:A:172:MET:HE1	1:A:204:ASN:OD1	2.15	0.46
1:A:44:ARG:HG3	1:A:44:ARG:NH1	2.30	0.46
1:B:239:LEU:HD22	1:B:239:LEU:N	2.31	0.45
1:B:101:VAL:HB	1:B:102:PRO:HD3	1.97	0.45
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.80	0.45
1:B:52:ASN:HD21	1:B:57:LEU:N	2.02	0.45
1:B:249:PHE:CD2	1:B:287:THR:HG22	2.52	0.45
1:A:86:ALA:O	1:A:94:THR:HG21	2.17	0.45
1:A:223:GLN:NE2	1:A:281:GLN:HE22	2.14	0.45
1:A:280:ILE:HG22	1:A:281:GLN:HE21	1.81	0.44
1:B:119:VAL:HG11	1:B:133:ILE:CD1	2.47	0.44
1:B:238:LYS:NZ	3:B:902:M0N:O6	2.51	0.44
1:A:52:ASN:HD21	1:A:57:LEU:N	2.01	0.44
1:A:203:ILE:HD12	1:A:203:ILE:HA	1.78	0.44
1:A:293:THR:O	1:A:297:ILE:HG13	2.17	0.44
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.83	0.43
3:A:901:M0N:H1	3:A:901:M0N:O	2.17	0.43
1:B:34:HIS:CE1	1:B:93:THR:O	2.71	0.43
1:B:55:MET:CE	1:B:190:SER:HB2	2.48	0.43
1:A:238:LYS:HB2	1:A:238:LYS:HE3	1.81	0.43
1:B:62:LEU:CD1	1:B:186:MET:HE3	2.49	0.43
1:B:122:LEU:HD13	1:B:189:LEU:HD11	2.01	0.43
1:A:244:VAL:O	1:A:248:ASN:ND2	2.50	0.43
1:B:60:ASP:HB2	4:B:549:HOH:O	2.18	0.43
1:A:245:HIS:HD2	1:A:289:SER:OG	2.02	0.43
1:B:5:LYS:O	1:B:5:LYS:HG2	2.19	0.43
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.90	0.42
1:B:52:ASN:C	1:B:54:VAL:N	2.77	0.42
1:B:152:TYR:CD2	1:B:152:TYR:C	2.97	0.42
1:B:32:TYR:O	1:B:35:ILE:HG22	2.19	0.42
1:A:32:TYR:CD1	1:A:111:MET:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:N	1:A:102:PRO:CD	2.83	0.42
1:A:7:GLU:HG3	1:B:303:MET:HE3	2.00	0.42
1:B:126:GLU:OE2	1:B:126:GLU:CA	2.67	0.42
1:B:249:PHE:HD2	1:B:287:THR:HG22	1.85	0.41
1:A:92:GLN:HG3	1:A:93:THR:N	2.36	0.41
1:B:203:ILE:HA	1:B:203:ILE:HD12	1.85	0.41
1:B:282:ILE:O	1:B:286:ASP:HB3	2.20	0.41
1:A:148:GLY:CA	1:B:28:ILE:HD11	2.51	0.41
1:B:157:LEU:CD1	1:B:158:PRO:HA	2.43	0.41
1:A:89:ARG:O	1:A:90:ARG:HB2	2.20	0.41
1:A:241:PHE:HB3	1:A:242:PRO:HD3	2.01	0.41
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.36	0.41
1:A:116:MET:CE	1:B:116:MET:SD	3.08	0.41
1:A:268:LEU:O	1:A:269:ARG:C	2.63	0.41
1:A:286:ASP:OD2	1:A:286:ASP:C	2.63	0.41
1:B:133:ILE:HD13	1:B:133:ILE:HA	1.91	0.40
1:B:200:VAL:O	1:B:203:ILE:HG22	2.21	0.40
1:A:90:ARG:HD3	1:A:90:ARG:HA	1.89	0.40
1:A:42:ASN:O	1:A:46:ASN:N	2.54	0.40
1:A:60:ASP:O	1:A:63:ALA:HB3	2.21	0.40
1:B:42:ASN:ND2	4:B:574:HOH:O	2.55	0.40
1:A:235:THR:O	1:A:269:ARG:HA	2.21	0.40
1:B:154:ARG:HD2	1:B:236:GLU:O	2.21	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	283/340 (83%)	274 (97%)	9 (3%)	0	100	100
1	B	282/340 (83%)	274 (97%)	7 (2%)	1 (0%)	30	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	565/680 (83%)	548 (97%)	16 (3%)	1 (0%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	LYS

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	272/317 (86%)	265 (97%)	7 (3%)	40 57
1	B	271/317 (86%)	262 (97%)	9 (3%)	33 48
All	All	543/634 (86%)	527 (97%)	16 (3%)	37 53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	79	ILE
1	A	94	THR
1	A	158	PRO
1	A	203	ILE
1	A	204	ASN
1	A	258	GLN
1	B	26	SER
1	B	28	ILE
1	B	90	ARG
1	B	92	GLN
1	B	141	ILE
1	B	251	LYS
1	B	252	THR
1	B	271	SER
1	B	281	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	52	ASN
1	A	61	GLN
1	A	85	ASN
1	A	109	ASN
1	A	121	GLN
1	A	130	HIS
1	A	137	ASN
1	A	144	HIS
1	A	164	GLN
1	A	204	ASN
1	A	211	GLN
1	A	245	HIS
1	A	258	GLN
1	A	281	GLN
1	A	288	ASN
1	A	298	ASN
1	A	299	GLN
1	A	306	ASN
1	B	24	ASN
1	B	34	HIS
1	B	46	ASN
1	B	52	ASN
1	B	96	HIS
1	B	109	ASN
1	B	121	GLN
1	B	137	ASN
1	B	147	GLN
1	B	204	ASN
1	B	223	GLN
1	B	255	GLN
1	B	259	HIS
1	B	281	GLN
1	B	288	ASN
1	B	298	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	M0N	A	901	2	20,21,21	2.70	8 (40%)	30,34,34	2.28	11 (36%)
3	M0N	B	902	2	20,21,21	2.72	9 (45%)	30,34,34	2.19	10 (33%)

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	M0N	A	901	2	-	0/23/23/23	0/2/2/2
3	M0N	B	902	2	-	2/23/23/23	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	M0N	P1-O3	6.82	1.61	1.50
3	B	902	M0N	P1-O3	6.81	1.61	1.50
3	B	902	M0N	P2-O6	6.64	1.61	1.50
3	A	901	M0N	P2-O6	6.53	1.61	1.50
3	A	901	M0N	C1-C2	-2.94	1.32	1.36
3	A	901	M0N	P2-C9	2.72	1.87	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	M0N	C1-C2	-2.67	1.33	1.36
3	B	902	M0N	P1-C9	2.63	1.87	1.85
3	A	901	M0N	P1-O2	-2.56	1.48	1.54
3	A	901	M0N	P2-O5	2.53	1.61	1.54
3	A	901	M0N	P2-O4	-2.50	1.48	1.54
3	B	902	M0N	P1-O1	2.50	1.61	1.54
3	B	902	M0N	P2-O5	2.49	1.61	1.54
3	B	902	M0N	P2-C9	2.47	1.86	1.85
3	B	902	M0N	P1-O2	-2.47	1.48	1.54
3	B	902	M0N	P2-O4	-2.42	1.48	1.54
3	A	901	M0N	P1-O1	2.38	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	M0N	C1-N1-C7	7.21	109.92	105.11
3	A	901	M0N	C1-N1-C7	6.97	109.76	105.11
3	A	901	M0N	N2-C7-N1	-4.76	107.40	111.02
3	B	902	M0N	N2-C7-N1	-4.08	107.91	111.02
3	B	902	M0N	C2-N2-C7	-3.77	104.77	107.09
3	A	901	M0N	C3-N2-C2	3.46	134.24	130.09
3	B	902	M0N	O4-P2-C9	3.07	112.94	106.19
3	A	901	M0N	O4-P2-C9	3.06	112.92	106.19
3	A	901	M0N	O5-P2-O6	-3.01	105.58	112.96
3	A	901	M0N	O1-P1-O3	-2.96	105.72	112.96
3	B	902	M0N	O5-P2-O6	-2.88	105.92	112.96
3	A	901	M0N	C2-N2-C7	-2.73	105.41	107.09
3	A	901	M0N	P2-C9-P1	-2.60	108.06	112.72
3	B	902	M0N	O2-P1-C9	2.59	111.88	106.19
3	B	902	M0N	C3-N2-C2	2.57	133.17	130.09
3	A	901	M0N	O2-P1-C9	2.54	111.78	106.19
3	A	901	M0N	O1-P1-O2	2.46	115.17	108.24
3	B	902	M0N	O6-P2-C9	-2.29	103.95	109.82
3	B	902	M0N	O3-P1-C9	-2.28	103.96	109.82
3	A	901	M0N	O4-P2-O5	2.07	114.08	108.24
3	B	902	M0N	O4-P2-O5	2.01	113.91	108.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	M0N	C1-C2-C8-C9

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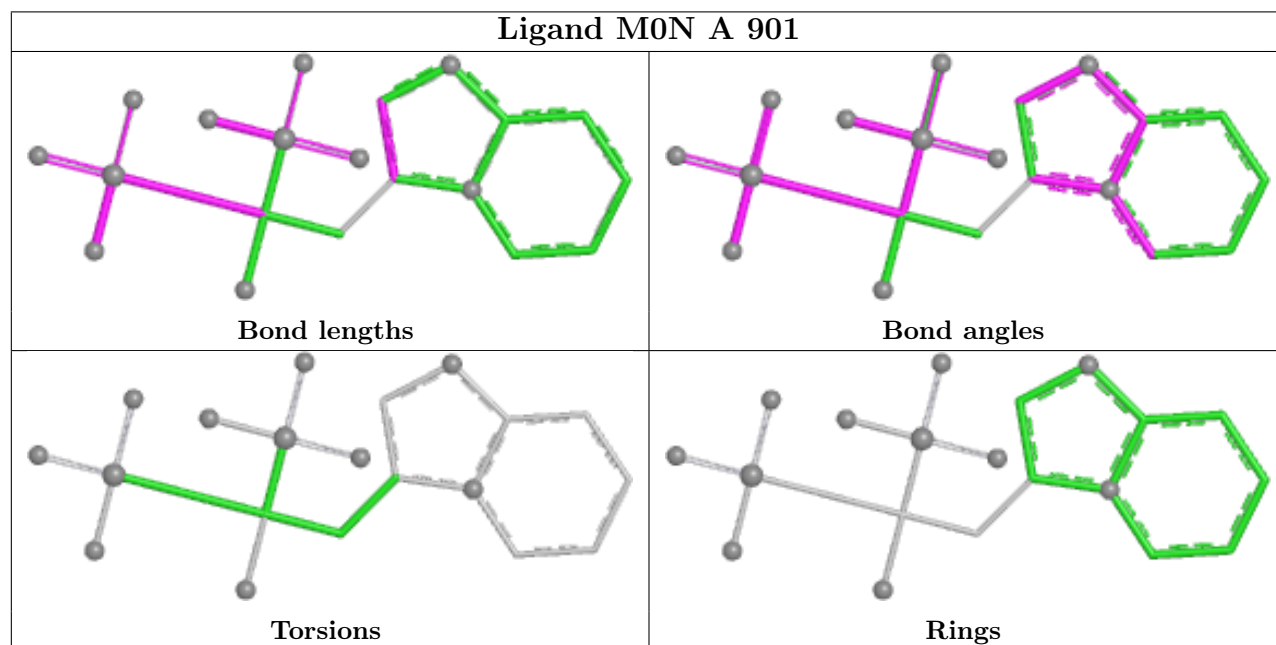
Mol	Chain	Res	Type	Atoms
3	B	902	M0N	N2-C2-C8-C9

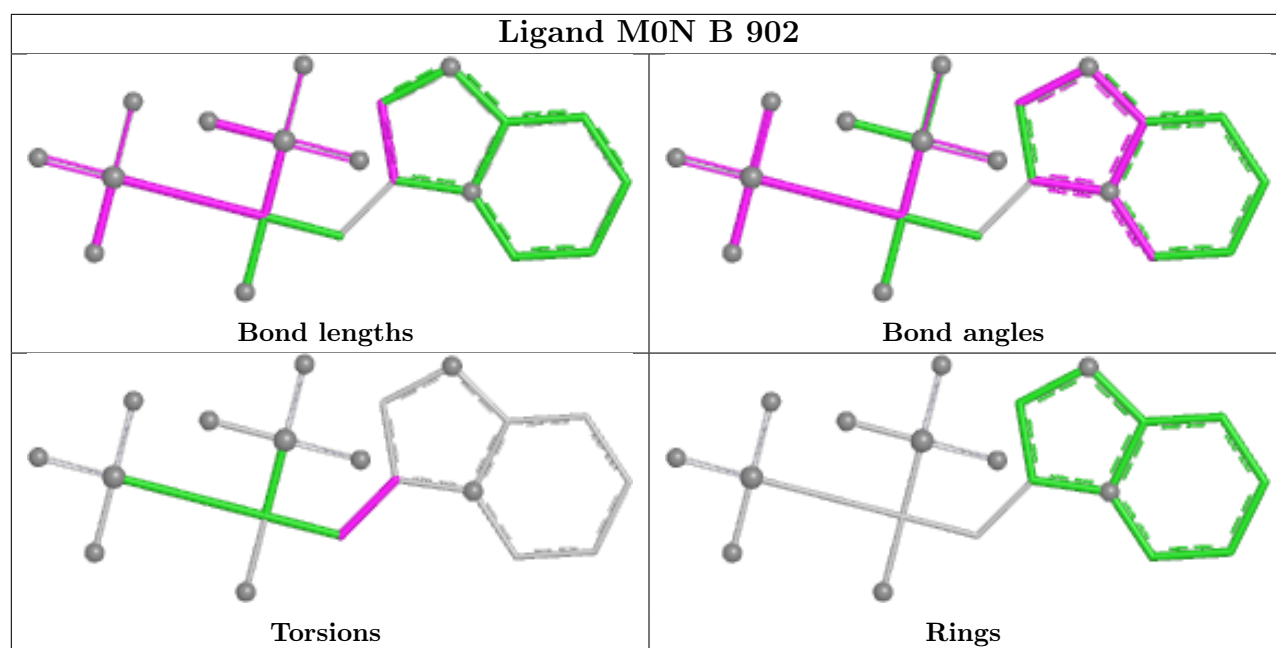
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	M0N	8	0
3	B	902	M0N	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	291/340 (85%)	-0.09	3 (1%) 79 81	27, 42, 74, 99	0
1	B	290/340 (85%)	0.10	3 (1%) 79 81	30, 47, 77, 95	0
All	All	581/680 (85%)	0.00	6 (1%) 79 81	27, 45, 77, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ASN	3.6
1	B	44	ARG	3.3
1	A	37	LEU	2.4
1	A	236	GLU	2.3
1	A	191	PRO	2.1
1	B	42	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

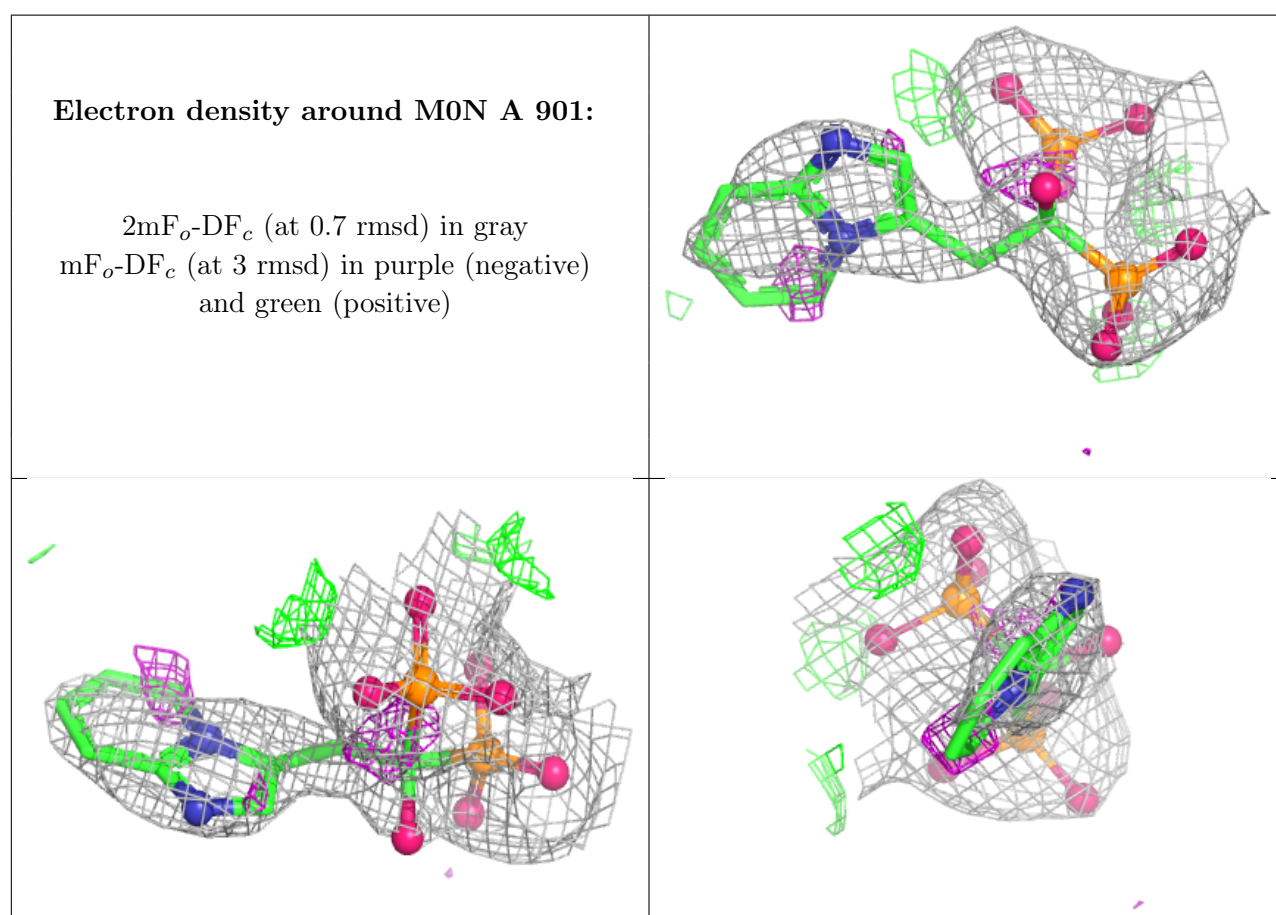
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

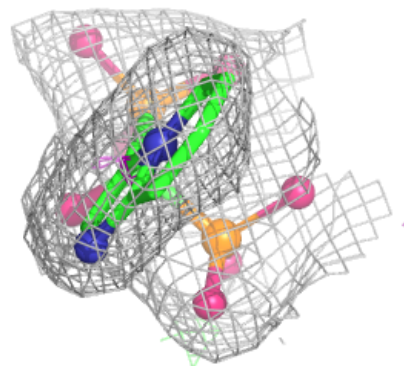
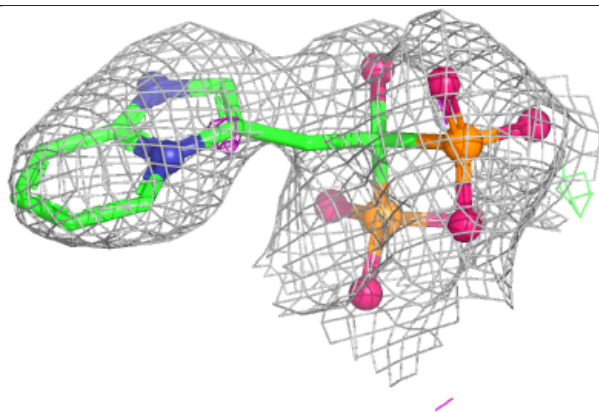
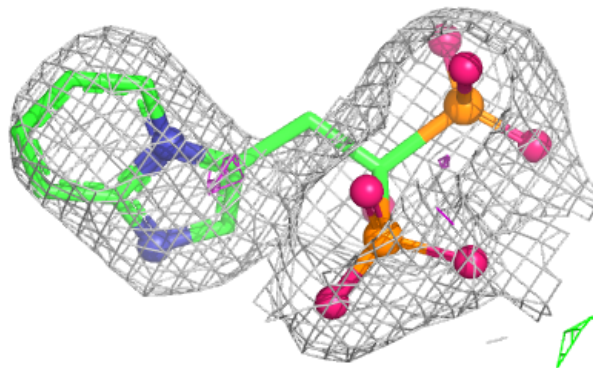
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1302	1/1	0.71	0.19	53,53,53,53	0
2	MG	A	1301	1/1	0.90	0.10	42,42,42,42	0
2	MG	B	1304	1/1	0.92	0.06	45,45,45,45	0
3	M0N	A	901	20/20	0.95	0.09	38,48,60,61	0
3	M0N	B	902	20/20	0.95	0.08	46,51,61,61	0
2	MG	B	1303	1/1	0.96	0.04	44,44,44,44	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 M0N B 902:

$2mF_o-DF_c$ (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.