



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:58 AM UTC

PDB ID : 2E91 / pdb_00002e91
Title : *S. cerevisiae* geranylgeranyl pyrophosphate synthase in complex with magnesium and BPH-91
Authors : Guo, R.T.; Ko, T.P.; Cao, R.; Chen, C.K.-M.; Jeng, W.Y.; Chang, T.H.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.
Deposited on : 2007-01-24
Resolution : 2.14 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)
Xtrriage (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

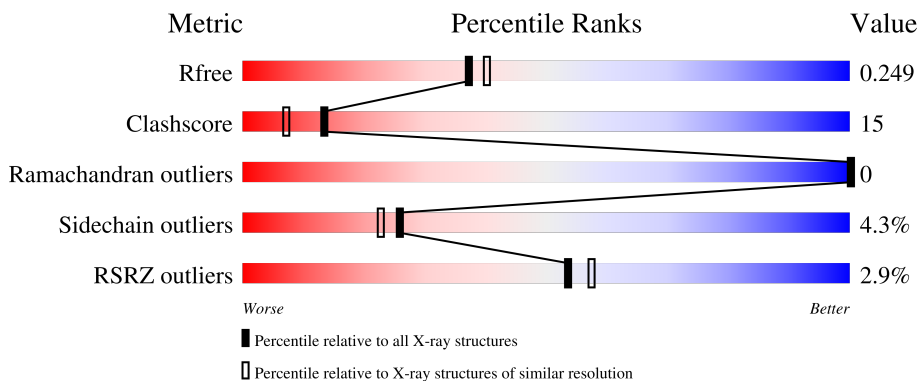
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	 3% 64% 21% 13%
1	B	340	 2% 61% 18% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5222 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
			Total	C	N	O	S			
1	A	296	2410	1548	409	443	10	0	0	0
1	B	283	2306	1483	388	426	9	0	0	0

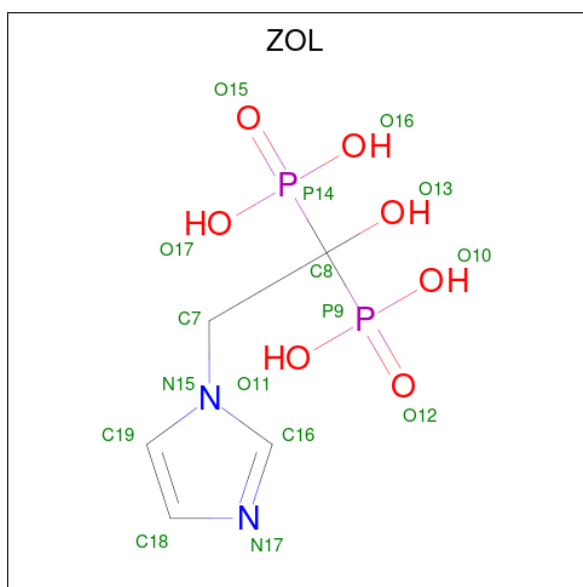
There are 10 discrepancies between the modelled and reference sequences:

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 ZOLEDRONIC ACID (CCD ID: ZOL) (formula: C₅H₁₀N₂O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	16	5	2	7	2	0	0
3	B	1	16	5	2	7	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total	O	0	0
			231	231		
4	B	239	Total	O	0	0
			239	239		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.66Å 116.29Å 126.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.14 30.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.14) 94.4 (30.00-2.14)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.14Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.249 0.197 , 0.249	Depositor DCC
R_{free} test set	1858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.633	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5222	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.03	1/2453 (0.0%)	1.16	15/3319 (0.5%)
1	B	0.98	1/2345 (0.0%)	1.13	9/3175 (0.3%)
All	All	1.01	2/4798 (0.0%)	1.15	24/6494 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-10.96	1.52	1.79
1	B	79	ILE	CA-CB	5.61	1.61	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	PHE	N-CA-C	7.77	122.02	112.23
1	A	82	ILE	N-CA-C	-6.93	104.02	110.53
1	A	101	VAL	CB-CA-C	-6.76	107.19	114.35
1	A	161	ILE	N-CA-C	-6.46	101.15	107.55
1	B	57	LEU	N-CA-C	-6.33	101.00	110.24
1	A	190	SER	N-CA-C	6.25	118.59	109.71
1	B	190	SER	N-CA-C	5.72	117.72	109.48
1	A	282	ILE	N-CA-C	-5.70	105.17	110.53
1	B	6	MET	N-CA-C	-5.67	105.01	111.14
1	B	270	THR	N-CA-C	5.55	119.14	110.32
1	A	38	LYS	CA-C-N	-5.51	115.08	120.98
1	A	38	LYS	C-N-CA	-5.51	115.08	120.98
1	A	23	GLN	N-CA-C	-5.35	105.36	111.14
1	B	59	LYS	N-CA-C	5.28	117.71	111.33
1	A	270	THR	N-CA-C	5.26	118.69	110.32
1	A	105	ILE	CB-CA-C	-5.24	105.27	111.97
1	A	54	VAL	CB-CA-C	-5.19	105.40	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	SER	N-CA-C	5.14	117.55	111.33
1	A	17	ASP	CA-C-N	-5.12	114.68	119.85
1	A	17	ASP	C-N-CA	-5.12	114.68	119.85
1	B	17	ASP	N-CA-C	-5.10	102.85	110.20
1	B	269	ARG	N-CA-C	-5.03	104.45	111.39
1	B	282	ILE	N-CA-C	-5.02	105.50	110.62
1	A	163	THR	N-CA-C	-5.02	102.58	110.36

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	2410	0	2466	82	0
1	B	2306	0	2363	72	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	16	0	7	0	0
3	B	16	0	7	2	0
4	A	231	0	0	6	0
4	B	239	0	0	10	0
All	All	5222	0	4843	141	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 (141) 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:163:THR:H	1:A:166:MET:HE3	0.93	1.07
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.33	1.06
1:A:163:THR:H	1:A:166:MET:CE	1.76	0.98
1:A:163:THR:N	1:A:166:MET:HE3	1.76	0.98
1:B:52:ASN:HD21	1:B:57:LEU:H	1.07	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:HD21	1:A:57:LEU:H	0.99	0.97
1:B:55:MET:HE2	1:B:187:GLU:HA	1.52	0.90
1:A:258:GLN:HE21	1:A:258:GLN:H	1.17	0.90
1:A:38:LYS:HE2	1:A:92:GLN:HB3	1.51	0.89
1:A:123:THR:HG21	1:A:128:LEU:CD2	2.04	0.87
1:B:5:LYS:CE	1:B:9:LYS:HE2	2.07	0.84
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.22	0.83
1:A:45:LEU:O	1:A:49:VAL:HG23	1.77	0.83
1:B:5:LYS:HE3	1:B:9:LYS:HE2	1.61	0.81
1:A:52:ASN:ND2	1:A:57:LEU:H	1.80	0.78
1:B:55:MET:CE	1:B:187:GLU:HA	2.15	0.76
1:A:140:LEU:O	1:A:144:HIS:HD2	1.70	0.74
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.70	0.73
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.36	0.73
1:B:52:ASN:ND2	1:B:57:LEU:H	1.86	0.73
1:A:183:LEU:HD21	1:A:199:LEU:HB2	1.70	0.72
1:A:56:ASN:HD22	1:A:192:SER:HB2	1.54	0.71
1:B:223:GLN:O	4:B:789:HOH:O	2.10	0.69
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.59	0.68
1:A:148:GLY:HA3	1:B:28:ILE:HD11	1.76	0.68
1:B:222:PHE:HB2	1:B:231:ALA:HB2	1.74	0.68
1:A:41:LYS:NZ	4:A:611:HOH:O	2.27	0.67
1:A:52:ASN:HD21	1:A:57:LEU:N	1.84	0.67
1:A:148:GLY:HA3	1:B:28:ILE:CD1	2.26	0.66
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.32	0.65
1:B:96:HIS:HE1	4:B:645:HOH:O	1.78	0.65
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.80	0.64
1:B:55:MET:HE3	1:B:190:SER:HB2	1.79	0.63
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.96	0.63
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.97	0.62
1:B:222:PHE:HE2	1:B:277:LEU:HG	1.63	0.61
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.83	0.60
1:A:38:LYS:HE2	1:A:92:GLN:CB	2.29	0.60
1:B:183:LEU:HD22	1:B:203:ILE:HB	1.81	0.60
1:B:5:LYS:HE2	1:B:9:LYS:HE2	1.81	0.60
3:B:902:ZOL:O12	4:B:651:HOH:O	2.16	0.60
1:A:38:LYS:HD2	1:A:89:ARG:O	2.02	0.59
1:A:34:HIS:HE1	1:A:93:THR:O	1.85	0.58
1:A:163:THR:N	1:A:166:MET:CE	2.51	0.58
1:A:258:GLN:HE21	1:A:258:GLN:N	1.96	0.58
3:B:902:ZOL:O16	4:B:651:HOH:O	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASP:OD2	4:B:651:HOH:O	2.18	0.57
1:A:273:LYS:HD3	4:A:866:HOH:O	2.04	0.57
1:A:6:MET:HE2	1:B:296:PHE:CE2	2.41	0.56
1:B:222:PHE:CE2	1:B:277:LEU:HG	2.40	0.56
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.04	0.56
1:B:45:LEU:O	1:B:49:VAL:HG23	2.06	0.56
1:B:23:GLN:H	1:B:23:GLN:CD	2.14	0.56
1:A:281:GLN:NE2	1:A:281:GLN:HA	2.21	0.56
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.54	0.55
1:A:163:THR:HG23	1:A:166:MET:CE	2.36	0.55
1:B:34:HIS:HE1	1:B:93:THR:O	1.90	0.54
1:B:96:HIS:HD2	4:B:811:HOH:O	1.89	0.54
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.72	0.54
1:A:183:LEU:HD21	1:A:199:LEU:CB	2.38	0.54
1:B:147:GLN:NE2	1:B:174:LYS:HG3	2.23	0.54
1:A:148:GLY:CA	1:B:28:ILE:HD11	2.38	0.54
1:A:145:ARG:HB3	1:B:20:TRP:CZ3	2.44	0.53
1:B:55:MET:HE2	1:B:187:GLU:CA	2.33	0.53
1:B:55:MET:HE3	1:B:190:SER:CB	2.38	0.53
1:A:273:LYS:HG3	1:A:274:ASP:N	2.24	0.53
1:A:229:GLY:N	4:A:705:HOH:O	2.42	0.52
1:A:139:GLU:HB2	1:A:181:LEU:HD22	1.92	0.52
1:A:116:MET:HG2	1:B:137:ASN:ND2	2.24	0.51
1:A:56:ASN:HD22	1:A:192:SER:CB	2.24	0.51
1:B:181:LEU:O	1:B:181:LEU:HD12	2.12	0.50
1:A:163:THR:HG23	1:A:166:MET:HE2	1.93	0.50
1:A:180:ARG:O	1:A:184:ARG:HG3	2.10	0.50
1:B:92:GLN:HG2	4:B:807:HOH:O	2.10	0.50
1:A:38:LYS:HD2	1:A:90:ARG:HB2	1.93	0.50
1:A:148:GLY:C	1:B:28:ILE:HD11	2.37	0.50
1:A:94:THR:HG22	1:A:96:HIS:CD2	2.46	0.50
1:B:222:PHE:O	1:B:223:GLN:C	2.56	0.49
1:B:22:SER:HB3	1:B:23:GLN:NE2	2.27	0.49
1:A:110:TYR:HE1	1:B:141:ILE:HG23	1.77	0.48
1:A:137:ASN:ND2	1:B:116:MET:HG2	2.28	0.48
1:B:157:LEU:HD12	1:B:158:PRO:HA	1.96	0.48
1:A:210:TYR:CD2	1:A:210:TYR:C	2.91	0.48
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.78	0.48
1:A:89:ARG:HD3	1:A:90:ARG:HD2	1.96	0.48
1:A:75:SER:OG	1:A:111:MET:HB2	2.13	0.47
1:A:163:THR:OG1	1:A:166:MET:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:NE2	4:B:808:HOH:O	2.47	0.47
1:A:223:GLN:HB2	1:A:280:ILE:HG21	1.95	0.47
1:A:89:ARG:HD3	1:A:90:ARG:CD	2.45	0.46
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.96	0.46
1:B:5:LYS:HA	1:B:5:LYS:HD2	1.64	0.46
1:B:258:GLN:HG2	1:B:286:ASP:OD2	2.16	0.46
1:B:251:LYS:HB2	1:B:251:LYS:HZ3	1.81	0.46
1:A:20:TRP:CH2	1:A:24:ASN:HB3	2.51	0.46
1:B:47:LEU:O	1:B:51:ILE:HG13	2.16	0.45
1:A:10:ILE:HG22	1:B:303:MET:HE1	1.98	0.45
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.79	0.45
1:A:185:LEU:O	1:A:189:LEU:HG	2.16	0.45
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.82	0.45
1:B:220:LYS:HA	1:B:220:LYS:HD2	1.80	0.45
1:B:147:GLN:HE21	1:B:174:LYS:HG3	1.81	0.45
1:A:144:HIS:HE1	4:A:815:HOH:O	2.00	0.45
1:A:6:MET:HE2	1:B:296:PHE:CD2	2.52	0.44
1:B:147:GLN:HE21	1:B:147:GLN:HA	1.83	0.44
1:B:284:GLU:HA	1:B:284:GLU:OE1	2.18	0.44
1:B:251:LYS:HD3	4:B:837:HOH:O	2.17	0.44
1:A:246:ALA:HB2	1:A:283:LEU:CD2	2.47	0.44
1:B:222:PHE:HD2	1:B:280:ILE:HD12	1.82	0.44
1:B:34:HIS:CE1	1:B:93:THR:O	2.70	0.43
1:A:132:LEU:HD11	1:A:189:LEU:HD21	1.99	0.43
1:B:181:LEU:HD12	1:B:181:LEU:C	2.43	0.43
1:A:34:HIS:CE1	1:A:93:THR:O	2.70	0.43
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.32	0.43
1:A:241:PHE:HB3	1:A:242:PRO:HD3	2.00	0.43
4:A:849:HOH:O	1:B:130:HIS:HE1	2.01	0.43
1:A:170:MET:SD	1:A:174:LYS:HD3	2.59	0.42
1:B:288:ASN:HD22	1:B:288:ASN:HA	1.59	0.42
1:A:140:LEU:O	1:A:144:HIS:CD2	2.62	0.42
1:A:148:GLY:HA3	1:B:28:ILE:HD12	1.99	0.42
1:A:94:THR:HG23	4:A:813:HOH:O	2.19	0.42
1:B:32:TYR:O	1:B:35:ILE:HG22	2.18	0.42
1:B:251:LYS:CE	4:B:837:HOH:O	2.67	0.42
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.34	0.42
1:A:280:ILE:HG22	1:A:281:GLN:HE21	1.84	0.42
1:A:58:PRO:HG2	1:A:61:GLN:HB2	2.01	0.42
1:A:101:VAL:N	1:A:102:PRO:CD	2.83	0.42
1:B:101:VAL:HB	1:B:102:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.36	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.89	0.41
1:A:281:GLN:NE2	1:A:281:GLN:CA	2.82	0.41
1:A:105:ILE:HD11	1:B:105:ILE:CD1	2.44	0.41
1:B:204:ASN:HD22	1:B:204:ASN:HA	1.66	0.41
1:A:113:PHE:CE2	1:B:140:LEU:HD13	2.56	0.41
1:B:61:GLN:NE2	1:B:189:LEU:HD22	2.35	0.41
1:B:154:ARG:HD2	1:B:236:GLU:O	2.20	0.41
1:A:10:ILE:HD13	1:A:10:ILE:HA	1.98	0.40
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.89	0.40
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.97	0.40
1:B:126:GLU:N	1:B:127:PRO:CD	2.85	0.40
1:B:292:TYR:CD1	1:B:292:TYR:C	2.99	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	290/340 (85%)	284 (98%)	6 (2%)	0	100	100
1	B	275/340 (81%)	273 (99%)	2 (1%)	0	100	100
All	All	565/680 (83%)	557 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	276/317 (87%)	267 (97%)	9 (3%)	33	33
1	B	265/317 (84%)	251 (95%)	14 (5%)	20	16
All	All	541/634 (85%)	518 (96%)	23 (4%)	26	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	57	LEU
1	A	60	ASP
1	A	181	LEU
1	A	203	ILE
1	A	225	SER
1	A	238	LYS
1	A	258	GLN
1	A	281	GLN
1	B	52	ASN
1	B	90	ARG
1	B	92	GLN
1	B	120	SER
1	B	125	LYS
1	B	141	ILE
1	B	147	GLN
1	B	181	LEU
1	B	203	ILE
1	B	238	LYS
1	B	251	LYS
1	B	258	GLN
1	B	283	LEU
1	B	288	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	52	ASN
1	A	56	ASN
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	96	HIS
1	A	106	ASN
1	A	109	ASN
1	A	137	ASN
1	A	144	HIS
1	A	204	ASN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	288	ASN
1	A	298	ASN
1	A	306	ASN
1	B	52	ASN
1	B	61	GLN
1	B	92	GLN
1	B	96	HIS
1	B	109	ASN
1	B	117	GLN
1	B	121	GLN
1	B	147	GLN
1	B	197	HIS
1	B	204	ASN
1	B	255	GLN
1	B	259	HIS
1	B	281	GLN
1	B	288	ASN
1	B	298	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	ZOL	A	901	2	16,16,16	1.70	6 (37%)	23,26,26	1.35	4 (17%)
3	ZOL	B	902	2	16,16,16	1.66	6 (37%)	23,26,26	1.28	3 (13%)

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	ZOL	A	901	2	-	2/23/23/23	0/1/1/1
3	ZOL	B	902	2	-	2/23/23/23	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZOL	P9-C8	3.09	1.87	1.85
3	A	901	ZOL	P14-O16	2.70	1.62	1.54
3	B	902	ZOL	P9-O11	2.49	1.61	1.54
3	B	902	ZOL	P9-C8	2.46	1.86	1.85
3	B	902	ZOL	P9-O10	2.46	1.61	1.54
3	B	902	ZOL	P14-O16	2.45	1.61	1.54
3	B	902	ZOL	P14-O17	2.44	1.61	1.54
3	A	901	ZOL	P9-O11	2.42	1.61	1.54
3	A	901	ZOL	P9-O10	2.40	1.61	1.54
3	A	901	ZOL	P14-O17	2.32	1.61	1.54
3	B	902	ZOL	P14-C8	2.26	1.86	1.85
3	A	901	ZOL	P14-C8	2.05	1.86	1.85

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	ZOL	P9-C8-P14	-4.15	105.28	112.72
3	A	901	ZOL	P9-C8-P14	-3.98	105.59	112.72
3	A	901	ZOL	C19-N15-C16	2.46	109.77	106.71
3	B	902	ZOL	C19-N15-C16	2.37	109.66	106.71
3	A	901	ZOL	N15-C16-N17	-2.24	106.13	111.45
3	B	902	ZOL	N15-C16-N17	-2.05	106.56	111.45
3	A	901	ZOL	C18-N17-C16	2.02	109.34	105.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

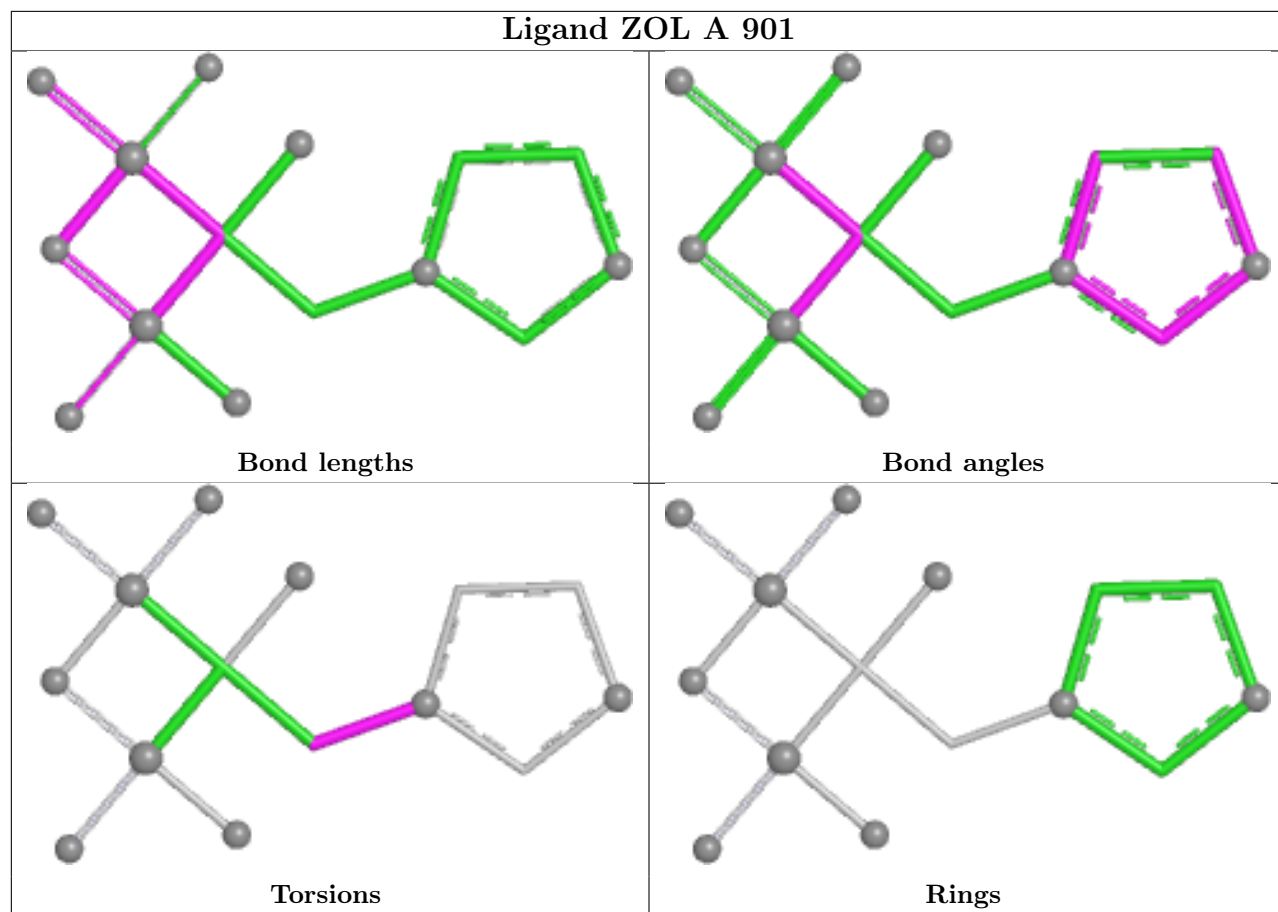
Mol	Chain	Res	Type	Atoms
3	B	902	ZOL	C8-C7-N15-C19
3	A	901	ZOL	C8-C7-N15-C16
3	A	901	ZOL	C8-C7-N15-C19
3	B	902	ZOL	C8-C7-N15-C16

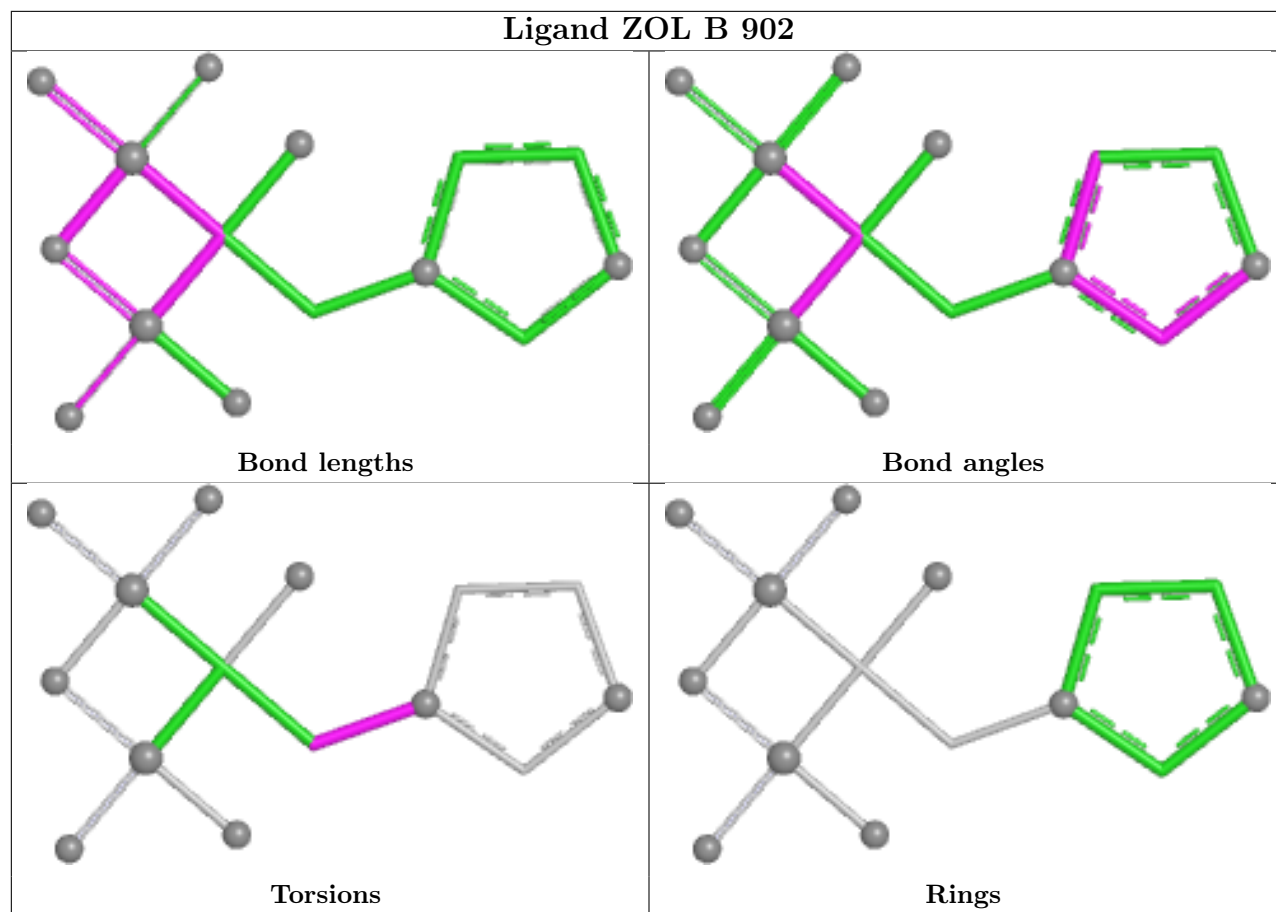
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	ZOL	2	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	296/340 (87%)	-0.04	10 (3%) 48 52	24, 37, 68, 89	0
1	B	283/340 (83%)	0.10	7 (2%) 58 62	27, 40, 63, 85	0
All	All	579/680 (85%)	0.03	17 (2%) 53 57	24, 39, 66, 89	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLY	3.6
1	A	230	PHE	3.0
1	A	90	ARG	2.9
1	B	192	SER	2.7
1	B	47	LEU	2.5
1	B	45	LEU	2.4
1	A	306	ASN	2.3
1	A	38	LYS	2.3
1	A	45	LEU	2.3
1	A	43	PHE	2.2
1	A	192	SER	2.2
1	B	222	PHE	2.1
1	B	277	LEU	2.1
1	B	223	GLN	2.1
1	A	304	ILE	2.1
1	B	126	GLU	2.1
1	A	41	LYS	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](#)

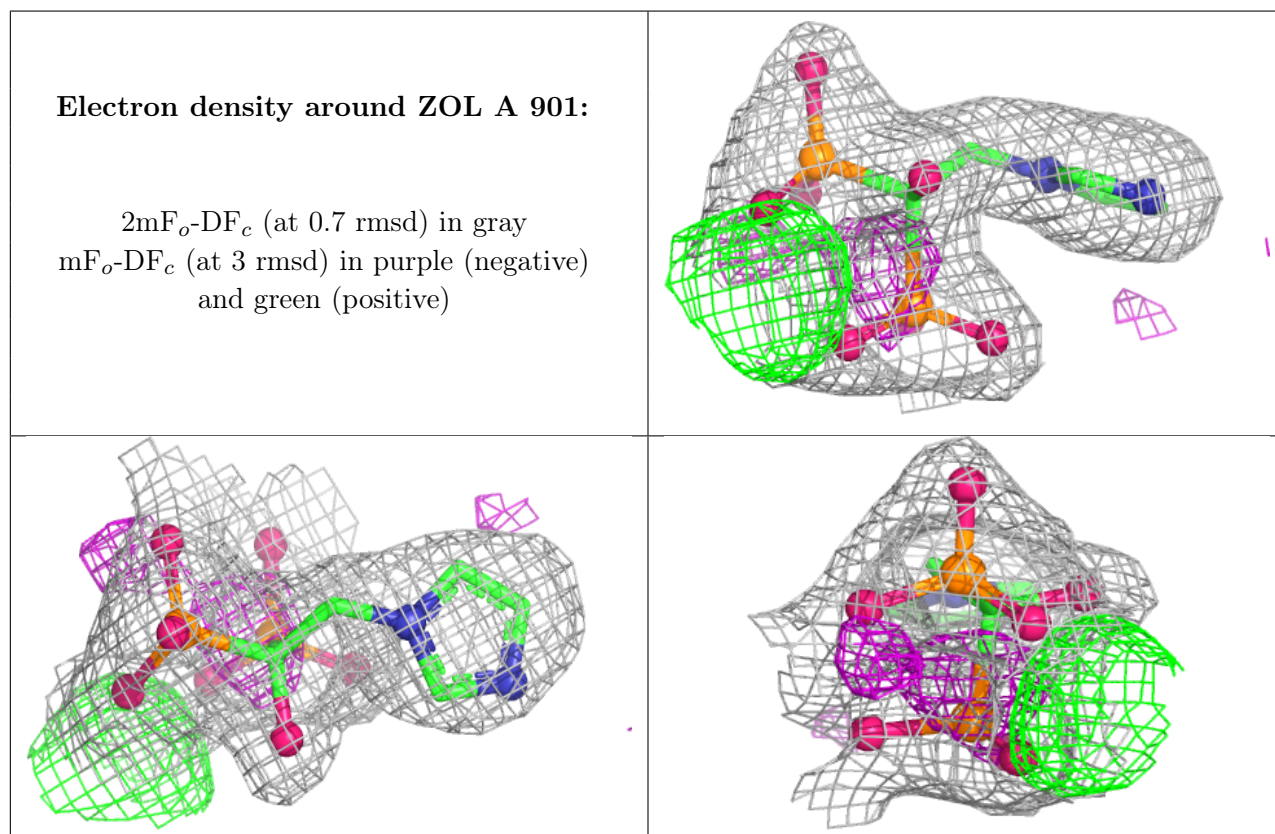
There are no oligosaccharides in this entry.

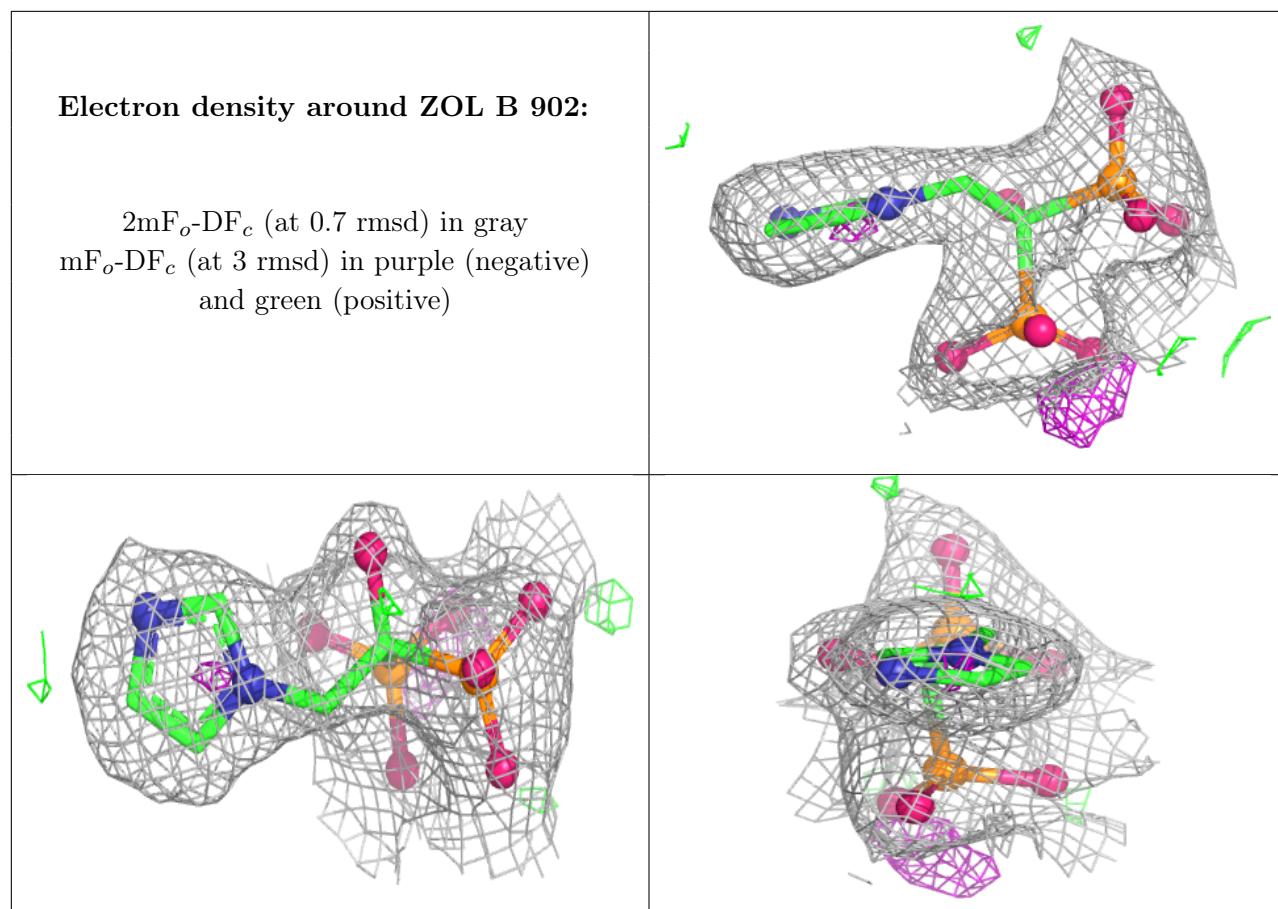
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	ZOL	A	901	16/16	0.92	0.09	30,36,40,41	0
2	MG	B	1303	1/1	0.94	0.04	39,39,39,39	0
3	ZOL	B	902	16/16	0.96	0.07	36,40,45,46	0
2	MG	A	1302	1/1	0.97	0.07	35,35,35,35	0
2	MG	A	1301	1/1	0.99	0.06	33,33,33,33	0
2	MG	B	1304	1/1	0.99	0.05	34,34,34,34	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.