



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:41 PM UTC

PDB ID : 2E95 / pdb\_00002e95  
Title : *S. cerevisiae* geranylgeranyl pyrophosphate synthase in complex with magnesium and BPH-675  
Authors : Guo, R.T.; Cao, R.; Ko, T.P.; Jeng, W.Y.; Chang, T.H.; Chen, C.K.-M.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.  
Deposited on : 2007-01-24  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

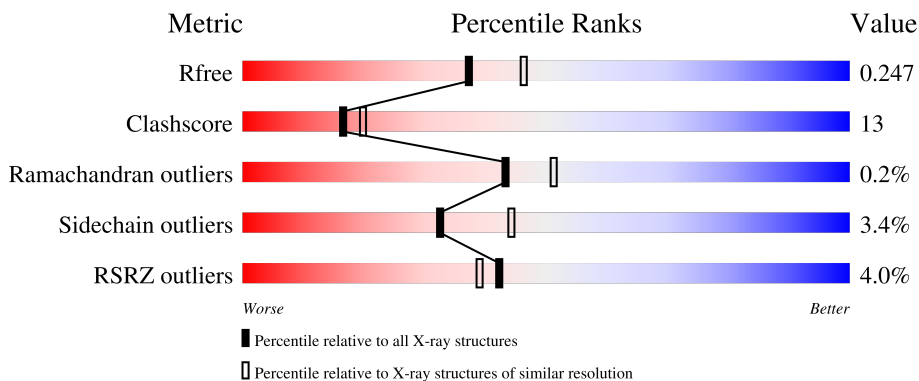
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	B75	A	1001	-	X	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5508 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	316	2581	1657	435	479	10	0	0	0
1	B	311	2539	1631	429	469	10	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		

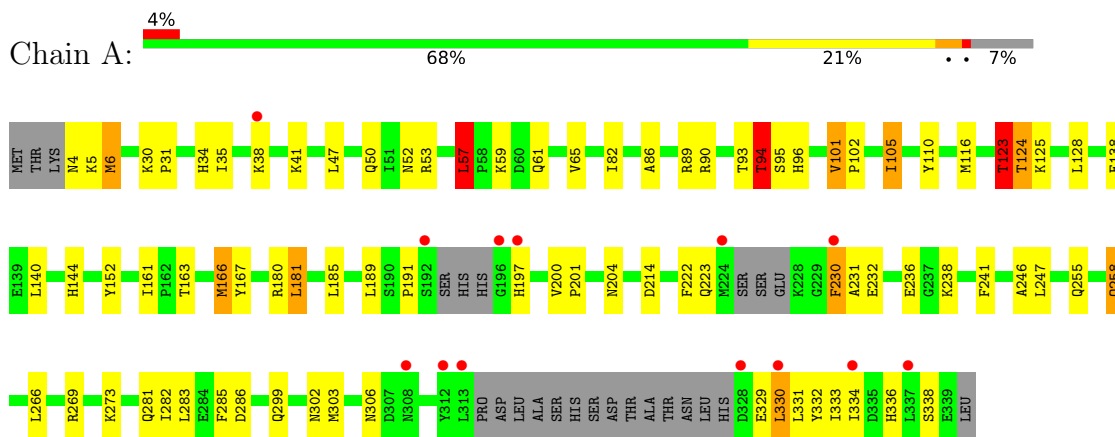
- Molecule 3 is 1-HYDROXY-2-[3'-(NAPHTHALENE-2-SULFONYLAMINO)-BIPHENYL-3-YL]ETHYLIDENE-1,1-BISPHOSPHONIC ACID (CCD ID: B75) (formula: C<sub>24</sub>H<sub>23</sub>NO<sub>9</sub>P<sub>2</sub>S).



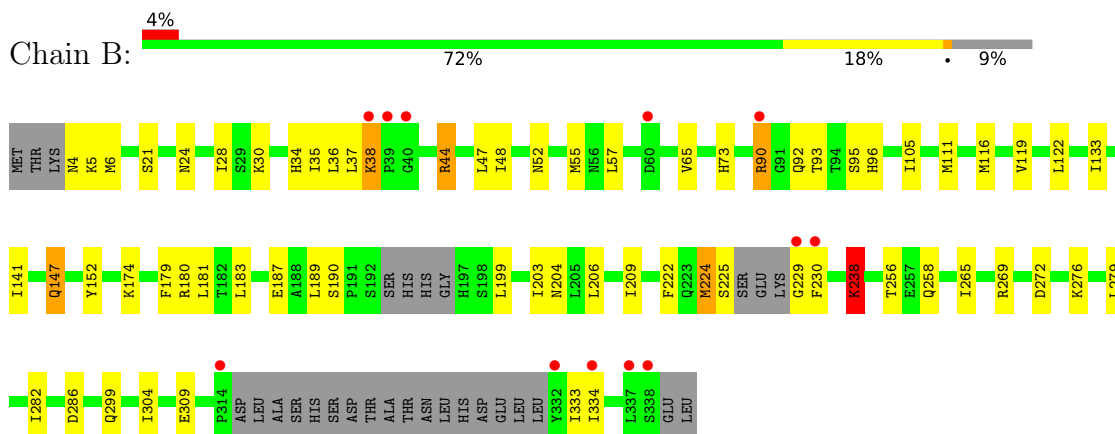
### 3 Residue-property plots [i](#)

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

- Molecule 1: Geranylgeranyl pyrophosphate synthetase



- 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, $\alpha$ , $\beta$ , $\gamma$	46.39Å 116.26Å 128.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.20 34.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (34.90-2.20) 95.3 (34.90-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.185 , 0.241 0.192 , 0.247	Depositor DCC
$R_{free}$ test set	1721 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.793	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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, B75

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	1.09	3/2626 (0.1%)	1.15	19/3551 (0.5%)
1	B	1.03	3/2585 (0.1%)	1.09	8/3498 (0.2%)
All	All	1.06	6/5211 (0.1%)	1.12	27/7049 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-14.04	1.44	1.79
1	B	105	ILE	CA-CB	6.42	1.61	1.54
1	B	111	MET	SD-CE	6.32	1.95	1.79
1	A	303	MET	SD-CE	5.46	1.93	1.79
1	A	241	PHE	CA-C	5.38	1.59	1.52
1	B	209	ILE	CA-CB	5.00	1.60	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LYS	N-CA-C	-7.76	102.45	112.23
1	B	65	VAL	N-CA-C	-7.59	103.39	110.53
1	B	256	THR	N-CA-C	6.90	119.39	111.11
1	A	161	ILE	CB-CA-C	-6.65	103.53	111.18
1	A	124	THR	N-CA-C	-6.63	105.48	113.97
1	A	105	ILE	CB-CA-C	-6.49	103.67	111.97
1	A	94	THR	N-CA-CB	-6.45	100.50	109.97
1	A	123	THR	CB-CA-C	-6.44	98.55	111.17
1	A	282	ILE	N-CA-C	-6.18	104.48	110.72
1	A	57	LEU	N-CA-C	-6.15	101.26	110.24
1	A	161	ILE	N-CA-C	-6.11	101.06	107.60
1	B	95	SER	N-CA-C	5.74	117.54	111.28
1	A	82	ILE	N-CA-C	-5.71	105.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	SER	N-CA-C	5.66	118.18	111.33
1	B	238	LYS	N-CA-C	5.61	118.79	110.48
1	A	191	PRO	N-CA-C	-5.53	105.35	114.75
1	A	65	VAL	N-CA-C	-5.46	105.05	110.62
1	A	138	GLU	N-CA-C	5.45	116.90	111.07
1	B	282	ILE	N-CA-C	-5.36	105.31	110.72
1	A	59	LYS	N-CA-C	5.31	117.82	111.71
1	A	94	THR	CB-CA-C	5.29	118.70	109.65
1	A	101	VAL	CB-CA-C	-5.27	108.76	114.35
1	B	224	MET	N-CA-C	-5.20	106.78	113.02
1	A	285	PHE	N-CA-C	5.14	119.68	113.41
1	A	231	ALA	N-CA-C	-5.11	104.34	111.39
1	B	269	ARG	N-CA-C	-5.05	104.42	111.39
1	B	44	ARG	N-CA-C	-5.01	105.73	111.14

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	2581	0	2627	83	0
1	B	2539	0	2585	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	2	0
3	B	37	0	19	9	0
4	A	169	0	0	4	0
4	B	168	0	0	5	0
All	All	5508	0	5231	134	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 13.

All (134) 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)
3:B:1002:B75:HAO	3:B:1002:B75:CAR	1.77	1.14
1:A:163:THR:H	1:A:166:MET:HE3	1.22	1.04
3:B:1002:B75:HAR	3:B:1002:B75:CAO	1.88	1.03
1:B:52:ASN:HD21	1:B:57:LEU:H	1.01	0.99
1:A:52:ASN:HD21	1:A:57:LEU:H	1.08	0.94
1:B:55:MET:HE2	1:B:187:GLU:HA	1.48	0.94
3:B:1002:B75:HAO	3:B:1002:B75:HAR	0.95	0.94
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.53	0.89
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.22	0.88
1:B:73:HIS:ND1	3:B:1002:B75:OAD	2.09	0.84
1:A:258:GLN:HE21	1:A:258:GLN:H	1.25	0.81
1:A:50:GLN:CD	1:A:329:GLU:HG2	2.06	0.81
1:A:35:ILE:HG13	1:A:38:LYS:HD2	1.61	0.80
1:A:38:LYS:HB3	1:A:90:ARG:HD3	1.65	0.78
1:B:36:LEU:C	1:B:38:LYS:H	1.92	0.77
1:B:52:ASN:ND2	1:B:57:LEU:H	1.79	0.77
1:A:50:GLN:CG	1:A:329:GLU:HG2	2.15	0.76
1:A:50:GLN:HG3	1:A:329:GLU:HG2	1.67	0.75
1:A:214:ASP:OD1	3:A:1001:B75:OAE	2.06	0.73
1:B:224:MET:O	1:B:225:SER:HB2	1.88	0.73
1:A:163:THR:N	1:A:166:MET:HE3	2.02	0.71
1:A:163:THR:HG23	1:A:166:MET:CE	2.21	0.71
1:A:52:ASN:ND2	1:A:57:LEU:H	1.87	0.70
1:A:38:LYS:HE3	1:A:89:ARG:O	1.92	0.69
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.38	0.69
1:B:47:LEU:HD13	1:B:333:ILE:HG21	1.75	0.68
1:A:123:THR:CG2	1:A:128:LEU:HD23	2.23	0.68
1:B:238:LYS:NZ	3:B:1002:B75:OAB	2.28	0.67
1:A:223:GLN:NE2	1:A:281:GLN:HE22	1.95	0.65
1:B:34:HIS:HE1	1:B:93:THR:O	1.80	0.65
1:B:4:ASN:ND2	4:B:557:HOH:O	2.30	0.65
1:A:94:THR:HG23	1:A:96:HIS:CD2	2.33	0.64
1:A:38:LYS:HE2	1:A:89:ARG:CG	2.27	0.64
1:A:330:LEU:CD1	1:A:330:LEU:H	2.12	0.62
1:B:333:ILE:HG13	4:B:654:HOH:O	1.98	0.62
1:A:232:GLU:O	1:A:236:GLU:HG3	1.99	0.62
1:B:119:VAL:HG11	1:B:133:ILE:HD13	1.81	0.62
1:A:34:HIS:HE1	1:A:93:THR:O	1.83	0.61
1:A:140:LEU:O	1:A:144:HIS:HD2	1.83	0.61
1:B:55:MET:CE	1:B:187:GLU:HA	2.28	0.61
1:A:181:LEU:HD12	1:A:181:LEU:O	2.01	0.60
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:O	1:A:334:ILE:HG13	2.02	0.59
1:B:52:ASN:HD21	1:B:57:LEU:N	1.86	0.58
1:A:302:ASN:HB3	1:A:306:ASN:ND2	2.19	0.58
1:B:286:ASP:OD1	1:B:286:ASP:C	2.45	0.57
1:B:179:PHE:CG	3:B:1002:B75:HAU	2.38	0.57
1:B:180:ARG:HH11	1:B:204:ASN:ND2	2.02	0.57
1:B:36:LEU:C	1:B:38:LYS:N	2.60	0.56
1:A:181:LEU:HD12	1:A:181:LEU:C	2.31	0.56
1:A:258:GLN:HE21	1:A:258:GLN:N	2.01	0.56
1:B:147:GLN:HE21	1:B:147:GLN:HA	1.70	0.56
1:A:4:ASN:OD1	4:A:717:HOH:O	2.18	0.55
1:A:116:MET:HE2	1:B:116:MET:SD	2.47	0.55
1:B:147:GLN:NE2	1:B:174:LYS:HD2	2.21	0.55
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.03	0.55
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.22	0.54
1:A:281:GLN:NE2	1:A:281:GLN:HA	2.22	0.54
1:A:144:HIS:HE1	4:B:707:HOH:O	1.90	0.54
1:A:38:LYS:CE	1:A:89:ARG:O	2.57	0.53
1:A:47:LEU:HD12	1:A:333:ILE:HD13	1.89	0.53
1:B:122:LEU:HD13	1:B:189:LEU:HD11	1.91	0.53
1:A:273:LYS:HD3	4:A:730:HOH:O	2.09	0.52
1:A:330:LEU:H	1:A:330:LEU:HD13	1.75	0.52
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.93	0.51
1:A:329:GLU:HG3	1:A:329:GLU:O	2.10	0.51
1:B:96:HIS:HD2	4:B:721:HOH:O	1.92	0.51
1:A:238:LYS:NZ	3:A:1001:B75:OAB	2.39	0.51
1:B:36:LEU:O	1:B:38:LYS:N	2.44	0.51
1:A:38:LYS:HE2	1:A:89:ARG:HG3	1.92	0.50
1:A:330:LEU:CD1	1:A:330:LEU:N	2.74	0.50
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.59	0.50
1:A:302:ASN:O	1:A:306:ASN:HB2	2.10	0.50
1:A:197:HIS:O	1:A:197:HIS:HD2	1.95	0.50
1:A:6:MET:HE3	1:B:299:GLN:CD	2.37	0.50
1:A:197:HIS:CD2	1:A:197:HIS:C	2.90	0.49
1:B:230:PHE:O	1:B:276:LYS:NZ	2.37	0.49
1:A:38:LYS:CB	1:A:90:ARG:HD3	2.39	0.48
1:A:152:TYR:OH	1:B:30:LYS:NZ	2.47	0.48
1:A:47:LEU:HD13	1:A:333:ILE:HG21	1.94	0.48
1:A:331:LEU:O	1:A:332:TYR:C	2.55	0.48
1:A:6:MET:HE3	1:B:299:GLN:OE1	2.13	0.48
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:NZ	4:A:605:HOH:O	2.35	0.47
1:A:30:LYS:HB2	1:A:31:PRO:HD3	1.95	0.47
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.79	0.47
1:A:96:HIS:HD2	4:A:661:HOH:O	1.97	0.47
1:A:185:LEU:O	1:A:189:LEU:HG	2.14	0.47
1:B:152:TYR:CD2	1:B:152:TYR:C	2.93	0.47
1:A:94:THR:CG2	1:A:96:HIS:NE2	2.78	0.46
1:B:222:PHE:HD1	1:B:229:GLY:O	1.99	0.46
1:A:163:THR:HG23	1:A:166:MET:HE1	1.98	0.46
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.97	0.46
1:B:55:MET:HE3	1:B:190:SER:HB2	1.96	0.46
1:B:48:ILE:HG13	3:B:1002:B75:HAM	1.97	0.46
1:A:86:ALA:O	1:A:94:THR:HG21	2.15	0.45
1:A:89:ARG:O	1:A:90:ARG:HB2	2.16	0.45
1:B:21:SER:H	1:B:24:ASN:HD22	1.63	0.45
1:B:5:LYS:HA	1:B:5:LYS:HD2	1.78	0.45
1:B:119:VAL:HG11	1:B:133:ILE:CD1	2.46	0.45
1:B:286:ASP:OD1	1:B:286:ASP:O	2.35	0.45
1:B:133:ILE:HG23	1:B:133:ILE:HD12	1.71	0.44
1:A:197:HIS:O	1:A:197:HIS:CD2	2.70	0.44
1:A:89:ARG:HG3	1:A:90:ARG:HD2	2.00	0.44
1:B:265:ILE:HG21	1:B:279:LEU:HB2	1.98	0.44
1:A:299:GLN:HB2	1:B:6:MET:HE1	2.00	0.43
1:A:255:GLN:NE2	1:A:286:ASP:OD2	2.41	0.43
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.85	0.43
1:A:330:LEU:N	1:A:330:LEU:HD12	2.33	0.43
1:A:222:PHE:HD1	1:A:230:PHE:HA	1.83	0.43
1:B:34:HIS:CE1	1:B:93:THR:O	2.65	0.43
1:A:101:VAL:O	1:A:105:ILE:HG13	2.18	0.43
1:B:55:MET:CE	1:B:187:GLU:HG2	2.49	0.42
1:B:258:GLN:HG2	1:B:286:ASP:OD2	2.19	0.42
1:A:266:LEU:O	1:A:269:ARG:NH1	2.52	0.42
1:B:44:ARG:HD2	3:B:1002:B75:OAD	2.19	0.42
1:A:222:PHE:CD1	1:A:230:PHE:HA	2.55	0.42
1:B:304:ILE:HD13	1:B:334:ILE:HD11	2.02	0.42
1:A:167:TYR:CD2	1:A:167:TYR:C	2.98	0.42
1:B:35:ILE:O	1:B:38:LYS:HB3	2.20	0.42
1:A:50:GLN:HG3	1:A:329:GLU:CG	2.43	0.41
1:A:50:GLN:HA	1:A:53:ARG:HD3	2.01	0.41
1:A:336:HIS:C	1:A:338:SER:H	2.28	0.41
1:B:90:ARG:N	1:B:90:ARG:HD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PHE:HA	3:B:1002:B75:HAU	2.02	0.41
1:B:183:LEU:HD21	1:B:199:LEU:C	2.45	0.41
1:B:272:ASP:OD1	1:B:272:ASP:C	2.63	0.41
1:A:110:TYR:HE1	1:B:141:ILE:HG23	1.86	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.95	0.41
1:A:101:VAL:N	1:A:102:PRO:CD	2.84	0.41
1:A:47:LEU:CD1	1:A:333:ILE:HD13	2.50	0.41
1:A:6:MET:HE1	1:B:299:GLN:HB2	2.02	0.40
1:B:225:SER:HB3	4:B:705:HOH:O	2.21	0.40
1:A:163:THR:CG2	1:A:166:MET:CE	2.98	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	308/340 (91%)	302 (98%)	6 (2%)	0	100	100
1	B	303/340 (89%)	298 (98%)	4 (1%)	1 (0%)	36	42
All	All	611/680 (90%)	600 (98%)	10 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	LEU

### 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	295/317 (93%)	284 (96%)	11 (4%)	30	41
1	B	291/317 (92%)	282 (97%)	9 (3%)	35	48
All	All	586/634 (92%)	566 (97%)	20 (3%)	32	44

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	57	LEU
1	A	61	GLN
1	A	94	THR
1	A	123	THR
1	A	124	THR
1	A	125	LYS
1	A	181	LEU
1	A	230	PHE
1	A	258	GLN
1	A	330	LEU
1	B	28	ILE
1	B	38	LYS
1	B	90	ARG
1	B	92	GLN
1	B	147	GLN
1	B	181	LEU
1	B	203	ILE
1	B	238	LYS
1	B	309	GLU

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
1	A	73	HIS
1	A	85	ASN
1	A	96	HIS

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	137	ASN
1	A	144	HIS
1	A	197	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	308	ASN
1	A	336	HIS
1	B	4	ASN
1	B	34	HIS
1	B	52	ASN
1	B	96	HIS
1	B	109	ASN
1	B	117	GLN
1	B	121	GLN
1	B	137	ASN
1	B	147	GLN
1	B	204	ASN
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	B75	B	1002	2	40,40,40	2.56	10 (25%)	62,62,62	2.33	11 (17%)
3	B75	A	1001	2	6,9,40	5.20	6 (100%)	12,15,62	2.01	3 (25%)

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	B75	B	1002	2	-	8/38/38/38	0/4/4/4
3	B75	A	1001	2	-	8/8/12/38	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	B75	PBJ-OAH	7.09	1.61	1.49
3	A	1001	B75	PBI-OAF	6.86	1.61	1.49
3	B	1002	B75	PBJ-OAH	6.70	1.61	1.50
3	B	1002	B75	PBI-OAF	6.35	1.60	1.50
3	B	1002	B75	CBB-NAZ	-6.22	1.33	1.43
3	B	1002	B75	OAC-SBK	6.03	1.50	1.43
3	B	1002	B75	OAD-SBK	5.96	1.50	1.43
3	A	1001	B75	PBI-OAA	-4.13	1.48	1.54
3	A	1001	B75	PBJ-OAB	-4.08	1.48	1.54
3	A	1001	B75	PBI-OAG	4.07	1.61	1.54
3	B	1002	B75	CBC-CBD	-4.03	1.39	1.49
3	A	1001	B75	PBJ-OAI	3.87	1.61	1.54
3	B	1002	B75	PBI-OAG	2.67	1.61	1.54
3	B	1002	B75	PBI-OAA	-2.52	1.48	1.54
3	B	1002	B75	PBJ-OAB	-2.50	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	B75	PBJ-OAI	2.35	1.61	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	B75	CBE-SBK-NAZ	11.30	120.90	106.88
3	B	1002	B75	OAD-SBK-OAC	-9.68	107.77	119.52
3	B	1002	B75	CAX-CBE-SBK	-4.73	116.14	120.07
3	A	1001	B75	OAA-PBI-CBH	4.36	117.24	106.08
3	B	1002	B75	CAR-CBE-SBK	3.92	124.07	119.76
3	A	1001	B75	OAG-PBI-CBH	-3.71	96.61	106.08
3	B	1002	B75	CBB-NAZ-SBK	3.43	133.59	122.94
3	B	1002	B75	PBJ-CBH-PBI	-2.83	107.65	112.72
3	A	1001	B75	OAI-PBJ-OAH	-2.53	107.11	113.45
3	B	1002	B75	OAA-PBI-CBH	2.44	111.56	106.19
3	B	1002	B75	OAD-SBK-CBE	-2.34	105.02	107.98
3	B	1002	B75	OAI-PBJ-OAH	-2.27	107.39	112.96
3	B	1002	B75	OAF-PBI-CBH	-2.07	104.52	109.82
3	B	1002	B75	CAO-CBB-NAZ	2.04	124.31	120.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

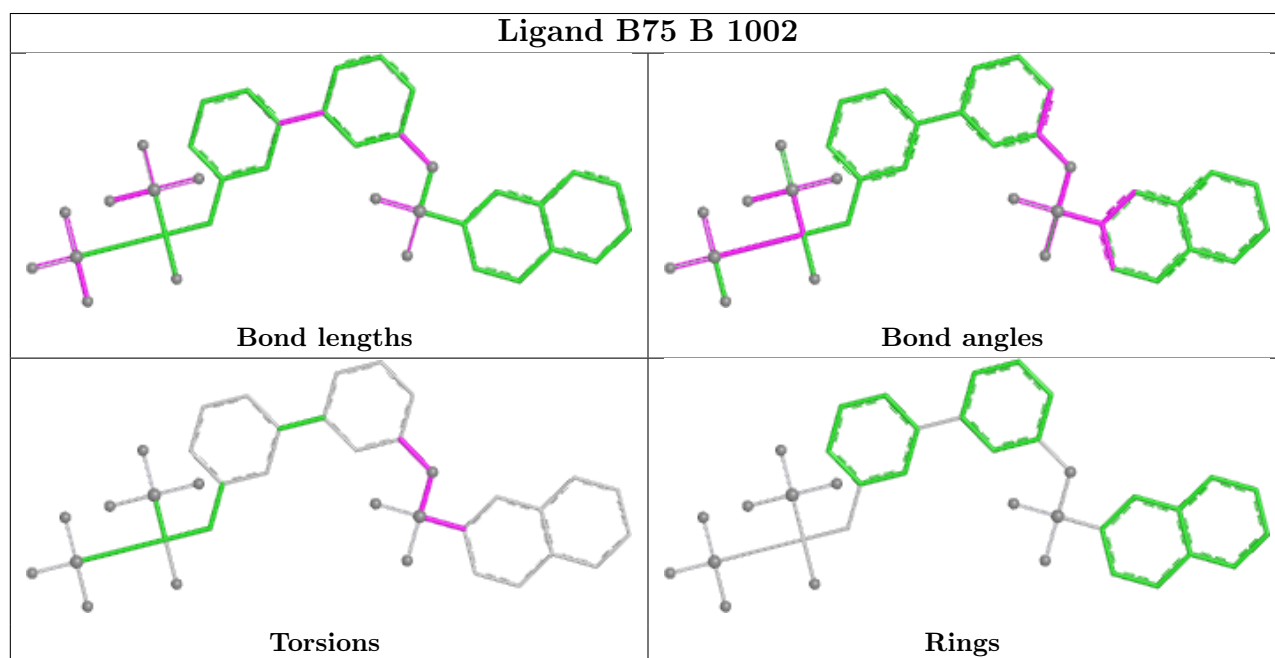
Mol	Chain	Res	Type	Atoms
3	A	1001	B75	PBJ-CBH-PBI-OAF
3	A	1001	B75	PBJ-CBH-PBI-OAA
3	A	1001	B75	OAE-CBH-PBI-OAF
3	A	1001	B75	PBI-CBH-PBJ-OAH
3	A	1001	B75	PBI-CBH-PBJ-OAI
3	A	1001	B75	OAE-CBH-PBJ-OAH
3	B	1002	B75	CBB-NAZ-SBK-CBE
3	B	1002	B75	CBB-NAZ-SBK-OAD
3	B	1002	B75	CBB-NAZ-SBK-OAC
3	B	1002	B75	CAX-CBE-SBK-NAZ
3	B	1002	B75	CAR-CBE-SBK-NAZ
3	B	1002	B75	CAR-CBE-SBK-OAC
3	A	1001	B75	PBJ-CBH-PBI-OAG
3	A	1001	B75	PBI-CBH-PBJ-OAB
3	B	1002	B75	CAX-CBE-SBK-OAC
3	B	1002	B75	CAO-CBB-NAZ-SBK

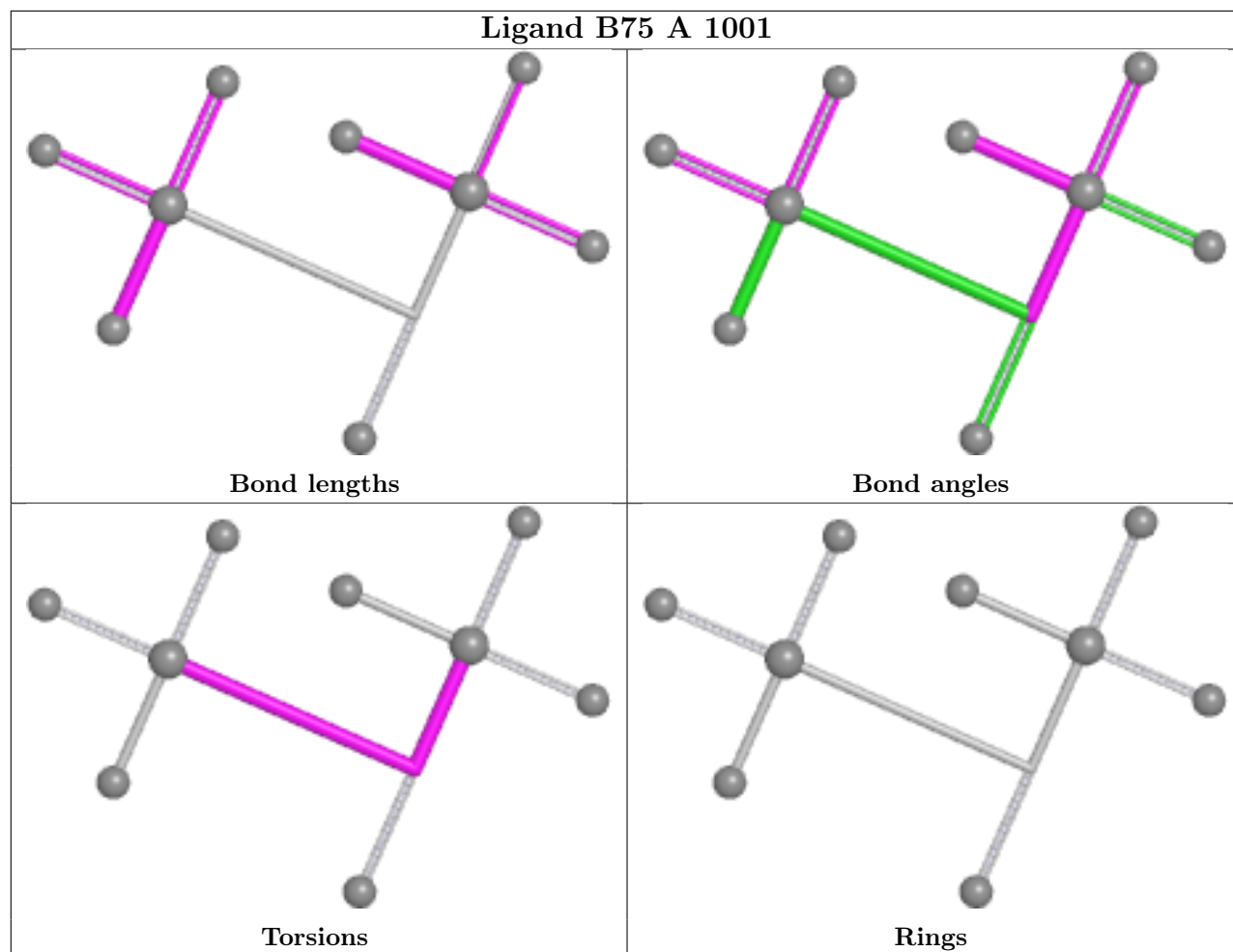
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	B75	9	0
3	A	1001	B75	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

### 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	316/340 (92%)	-0.14	13 (4%) 41 38	21, 33, 84, 112	0
1	B	311/340 (91%)	-0.08	12 (3%) 43 40	21, 34, 73, 97	0
All	All	627/680 (92%)	-0.11	25 (3%) 42 39	21, 34, 81, 112	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	SER	3.7
1	A	196	GLY	3.6
1	A	313	LEU	3.4
1	B	39	PRO	3.3
1	A	192	SER	3.1
1	A	330	LEU	3.0
1	A	197	HIS	3.0
1	B	40	GLY	3.0
1	A	312	TYR	2.8
1	A	334	ILE	2.7
1	A	230	PHE	2.6
1	A	328	ASP	2.6
1	B	332	TYR	2.4
1	B	337	LEU	2.4
1	B	60	ASP	2.3
1	B	90	ARG	2.3
1	A	308	ASN	2.2
1	B	229	GLY	2.2
1	B	314	PRO	2.2
1	A	337	LEU	2.2
1	A	38	LYS	2.1
1	B	230	PHE	2.1
1	B	38	LYS	2.1
1	A	224	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	334	ILE	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](#)

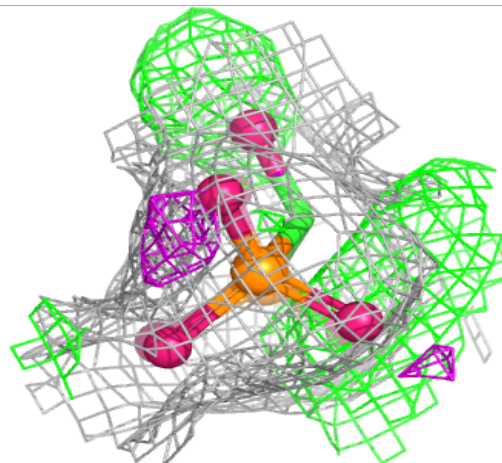
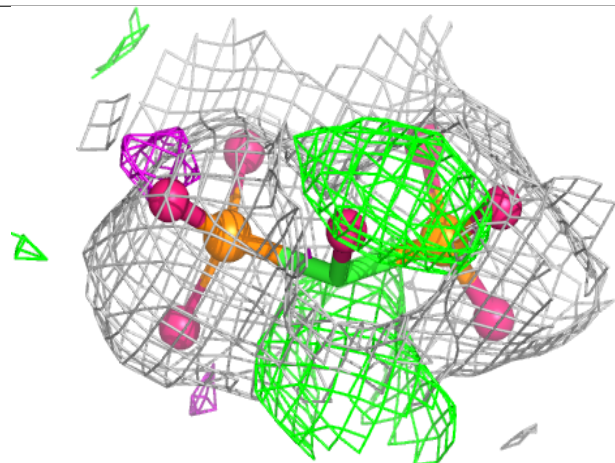
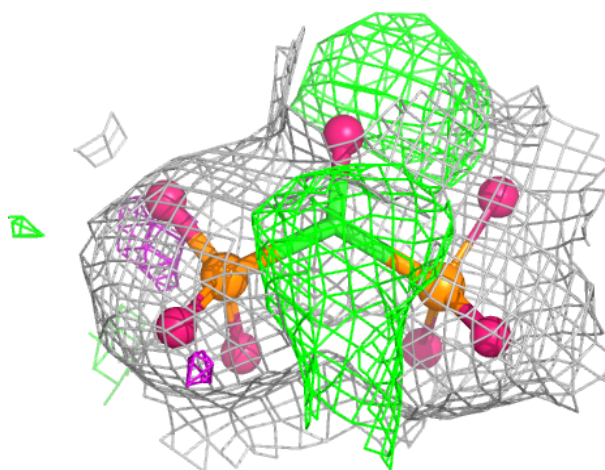
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

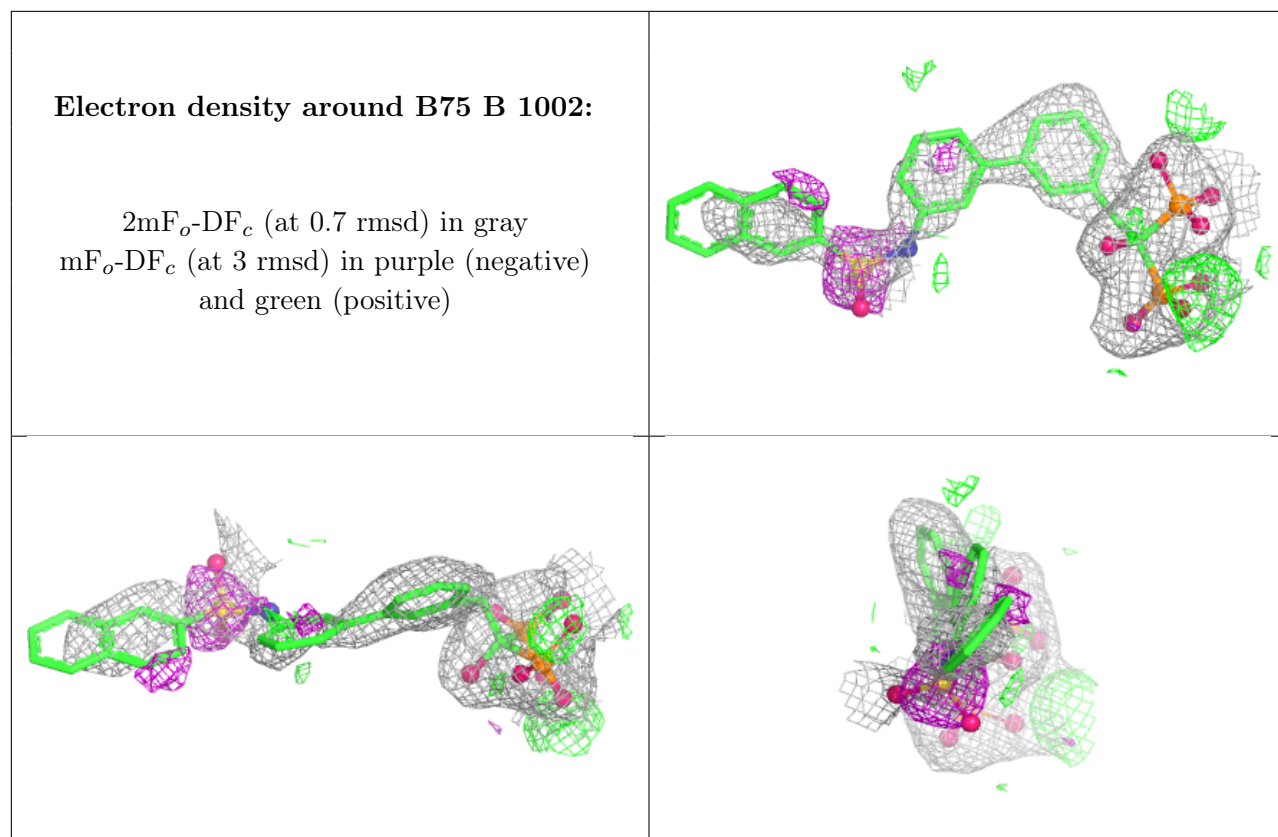
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1301	1/1	0.86	0.12	36,36,36,36	0
3	B75	A	1001	10/37	0.87	0.12	38,42,48,48	0
3	B75	B	1002	37/37	0.92	0.15	35,70,96,96	0
2	MG	B	1304	1/1	0.93	0.07	30,30,30,30	0
2	MG	B	1303	1/1	0.97	0.03	34,34,34,34	0
2	MG	A	1302	1/1	0.98	0.06	29,29,29,29	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 B75 A 1001:**

$2mF_o-DF_c$  (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.