



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 1N24 / pdb_00001n24
Title : (+)-Bornyl diphosphate synthase: Complex with Mg and product
Authors : Whittington, D.A.; Wise, M.L.; Urbansky, M.; Coates, R.M.; Croteau, R.B.; Christianson, D.W.
Deposited on : 2002-10-21
Resolution : 2.30 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

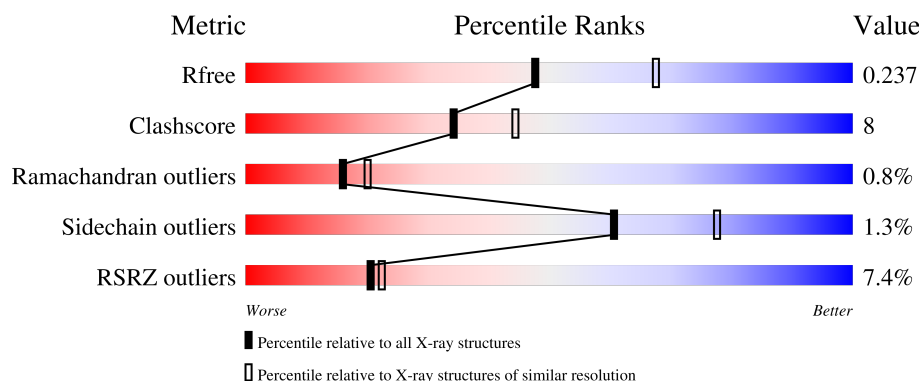
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	549	 6% 80% 16% . .
1	B	549	 8% 78% 17% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9146 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.

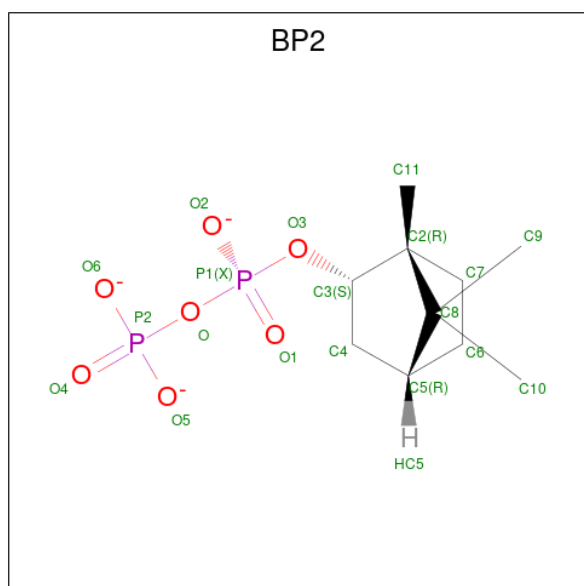
- Molecule 1 is a protein called (+)-bornyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4408	2859	731	801	17			
1	B	527	Total	C	N	O	S	0	0	0
			4346	2817	717	794	18			

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

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

- Molecule 3 is (+)-BORNYL DIPHOSPHATE (CCD ID: BP2) (formula: C₁₀H₁₇O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			19	10	7	2		
3	B	1	Total	C	O	P	0	0
			19	10	7	2		

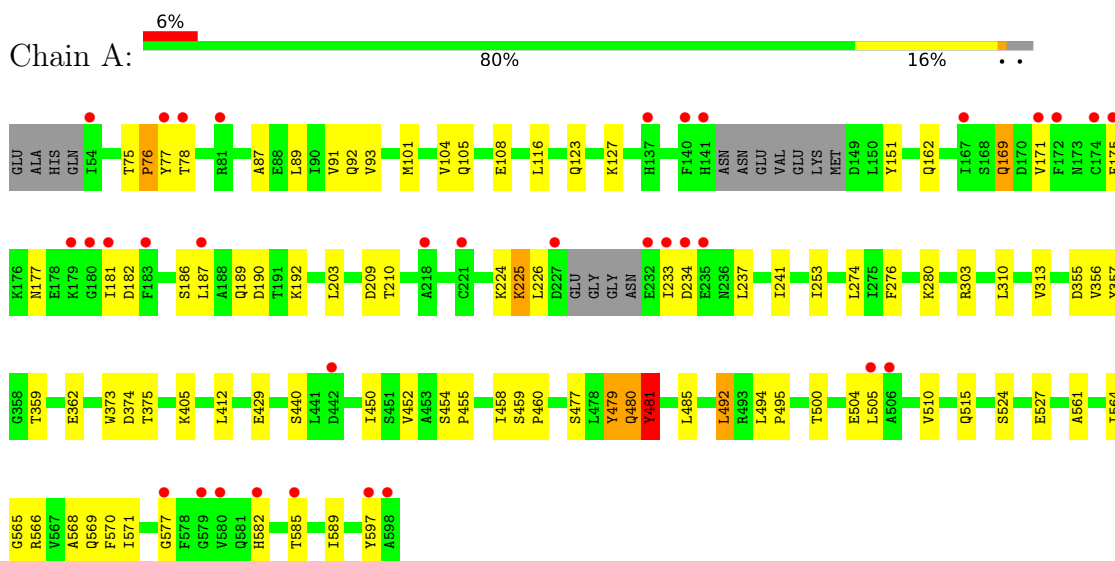
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	157	Total	O	0	0
			157	157		

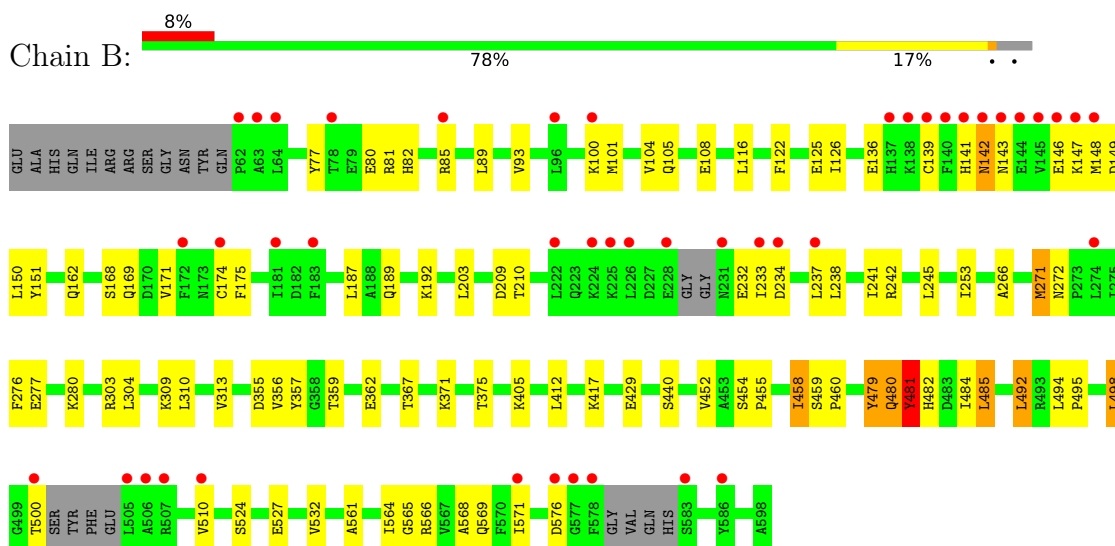
3 Residue-property plots

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: (+)-bornyl diphosphate synthase



• Molecule 1: (+)-bornyl diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.20Å 117.53Å 120.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.30) 94.9 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.238 0.210 , 0.237	Depositor DCC
R_{free} test set	2465 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9146	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, BP2

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	0.48	3/4527 (0.1%)	0.90	16/6135 (0.3%)
1	B	0.42	1/4460 (0.0%)	0.87	9/6042 (0.1%)
All	All	0.46	4/8987 (0.0%)	0.89	25/12177 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PRO	CA-C	-10.97	1.36	1.52
1	A	75	THR	C-N	6.30	1.41	1.34
1	A	169	GLN	CD-OE1	5.05	1.33	1.23
1	B	100	LYS	C-N	-5.01	1.27	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	GLN	N-CA-C	-13.30	97.05	113.01
1	A	480	GLN	N-CA-C	-12.05	97.83	112.54
1	A	76	PRO	CA-N-CD	-10.66	97.08	112.00
1	B	189	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	A	76	PRO	CB-CA-C	-9.12	98.88	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	TYR	N-CA-C	7.58	122.35	113.18
1	A	357	TYR	N-CA-C	7.41	122.71	112.04
1	B	440	SER	N-CA-C	-7.31	101.10	110.53
1	A	78	THR	N-CA-C	-7.24	104.06	114.12
1	A	458	ILE	N-CA-C	6.77	116.89	110.53
1	B	458	ILE	N-CA-C	6.68	116.81	110.53
1	B	357	TYR	N-CA-C	6.67	121.72	112.45
1	B	189	GLN	CG-CD-NE2	6.64	126.36	116.40
1	A	440	SER	N-CA-C	-6.53	101.91	110.53
1	A	75	THR	CA-C-N	6.22	125.63	118.85
1	A	75	THR	C-N-CA	6.22	125.63	118.85
1	A	116	LEU	N-CA-C	-6.19	105.38	113.17
1	A	76	PRO	O-C-N	-6.12	114.58	122.23
1	A	76	PRO	CA-C-O	6.07	128.54	119.74
1	A	76	PRO	N-CA-C	-6.00	105.35	113.40
1	B	116	LEU	N-CA-C	-5.93	105.69	113.17
1	A	479	TYR	N-CA-C	5.87	120.29	113.18
1	B	100	LYS	CA-C-O	-5.83	114.74	121.15
1	A	450	ILE	N-CA-C	-5.43	107.14	111.81
1	A	481	TYR	N-CA-C	-5.25	99.61	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	481	TYR	Sidechain
1	B	481	TYR	Sidechain

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	4408	0	4293	64	0
1	B	4346	0	4236	70	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	19	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	17	0	0
4	A	191	0	0	5	0
4	B	157	0	0	3	0
All	All	9146	0	8563	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (132) 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:429:GLU:HB3	1:A:510:VAL:HG21	1.28	1.13
1:B:429:GLU:HB3	1:B:510:VAL:HG21	1.28	1.13
1:B:146:GLU:HG2	1:B:147:LYS:H	1.22	1.05
1:B:148:MET:HE2	1:B:174:CYS:HB3	1.45	0.97
1:B:141:HIS:O	1:B:142:ASN:OD1	1.86	0.93
1:A:101:MET:HE2	1:A:105:GLN:HB3	1.48	0.91
1:B:143:ASN:OD1	1:B:171:VAL:HG22	1.73	0.88
1:B:492:LEU:HD13	1:B:568:ALA:HB2	1.55	0.88
1:A:310:LEU:O	1:A:313:VAL:HG22	1.81	0.80
1:A:492:LEU:HD13	1:A:568:ALA:HB2	1.62	0.80
1:B:143:ASN:HD21	1:B:168:SER:HB3	1.50	0.76
1:B:143:ASN:OD1	1:B:171:VAL:CG2	2.34	0.76
1:A:429:GLU:CB	1:A:510:VAL:HG21	2.14	0.75
1:B:146:GLU:HG2	1:B:147:LYS:N	2.02	0.72
1:B:141:HIS:O	1:B:142:ASN:CG	2.33	0.71
1:A:101:MET:HE2	1:A:105:GLN:CB	2.21	0.68
1:B:479:TYR:C	1:B:481:TYR:H	1.96	0.67
1:B:479:TYR:C	1:B:481:TYR:N	2.43	0.67
1:B:81:ARG:HH12	1:B:82:HIS:CE1	2.12	0.66
1:B:143:ASN:ND2	1:B:168:SER:HB3	2.10	0.66
1:A:494:LEU:HB2	1:A:495:PRO:HD3	1.77	0.66
1:B:276:PHE:CZ	1:B:280:LYS:HD2	2.30	0.66
1:A:224:LYS:C	1:A:226:LEU:H	2.05	0.65
1:B:494:LEU:HB2	1:B:495:PRO:HD3	1.77	0.65
1:A:225:LYS:HE3	1:A:233:ILE:HD11	1.80	0.64
1:B:498:LEU:HD13	1:B:532:VAL:HG11	1.80	0.63
1:B:238:LEU:O	1:B:242:ARG:HG3	1.99	0.62
1:A:123:GLN:O	1:A:127:LYS:HG3	2.00	0.62
1:A:429:GLU:HB3	1:A:510:VAL:CG2	2.17	0.62
1:B:492:LEU:HD12	1:B:492:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PHE:CZ	1:A:280:LYS:HD2	2.35	0.60
1:A:92:GLN:HB3	1:A:274:LEU:HD13	1.83	0.60
1:B:266:ALA:HB2	1:B:276:PHE:CE1	2.37	0.59
1:A:189:GLN:HG3	1:A:190:ASP:N	2.17	0.59
1:A:452:VAL:HG22	1:A:492:LEU:HG	1.84	0.59
1:B:169:GLN:NE2	1:B:210:THR:HB	2.18	0.59
1:A:585:THR:HG22	1:A:589:ILE:HG13	1.84	0.58
1:B:81:ARG:NH1	1:B:82:HIS:CE1	2.72	0.56
1:B:452:VAL:HG22	1:B:492:LEU:HG	1.86	0.56
1:B:175:PHE:HB3	1:B:187:LEU:HD11	1.88	0.56
1:B:276:PHE:CE2	1:B:280:LYS:HD2	2.41	0.56
1:A:515:GLN:H	1:A:515:GLN:CD	2.15	0.55
1:A:479:TYR:C	1:A:481:TYR:N	2.54	0.55
1:B:500:THR:HG22	1:B:576:ASP:HB2	1.88	0.55
1:B:104:VAL:O	1:B:108:GLU:HG3	2.07	0.54
1:A:510:VAL:HG23	4:A:815:HOH:O	2.06	0.54
1:B:492:LEU:HD13	1:B:568:ALA:CB	2.35	0.54
1:A:104:VAL:O	1:A:108:GLU:HG3	2.07	0.54
1:B:253:ILE:HD11	1:B:566:ARG:HB2	1.90	0.53
1:B:452:VAL:CG2	1:B:492:LEU:HG	2.37	0.53
1:A:355:ASP:OD1	1:A:356:VAL:HG23	2.08	0.53
1:A:303:ARG:NH2	4:A:990:HOH:O	2.28	0.53
1:A:373:TRP:HB2	4:A:912:HOH:O	2.08	0.53
1:A:452:VAL:CG2	1:A:492:LEU:HG	2.39	0.53
1:A:500:THR:O	1:A:504:GLU:HG3	2.09	0.53
1:A:233:ILE:HG22	1:A:234:ASP:N	2.23	0.53
1:A:454:SER:HB2	1:A:455:PRO:HD3	1.91	0.52
1:B:417:LYS:HG3	4:B:839:HOH:O	2.10	0.52
1:A:189:GLN:HG3	1:A:190:ASP:H	1.75	0.52
1:A:224:LYS:C	1:A:226:LEU:N	2.68	0.52
1:A:186:SER:O	1:A:189:GLN:HG2	2.10	0.51
1:B:89:LEU:O	1:B:93:VAL:HG23	2.10	0.51
1:A:280:LYS:HG2	1:A:597:TYR:CD2	2.46	0.51
1:A:253:ILE:HD11	1:A:566:ARG:HB2	1.92	0.50
1:A:480:GLN:O	1:A:481:TYR:HB2	2.11	0.50
1:A:181:ILE:HG22	1:A:182:ASP:OD1	2.11	0.50
1:A:375:THR:HB	1:B:412:LEU:HD23	1.93	0.50
1:A:570:PHE:HB2	4:A:858:HOH:O	2.11	0.50
1:B:233:ILE:O	1:B:234:ASP:C	2.53	0.50
1:B:169:GLN:HE22	1:B:210:THR:H	1.60	0.49
1:A:225:LYS:CE	1:A:233:ILE:HD11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:O	1:B:233:ILE:HG13	2.12	0.49
1:A:280:LYS:HE3	1:A:597:TYR:HD2	1.78	0.48
1:B:310:LEU:O	1:B:313:VAL:HG22	2.13	0.48
1:A:175:PHE:HB3	1:A:187:LEU:HD11	1.95	0.48
1:B:355:ASP:OD1	1:B:356:VAL:HG23	2.13	0.48
1:A:429:GLU:O	1:A:510:VAL:HG22	2.14	0.48
1:B:524:SER:OG	1:B:527:GLU:HG3	2.14	0.48
1:B:454:SER:HB2	1:B:455:PRO:HD3	1.95	0.47
1:B:125:GLU:OE1	1:B:125:GLU:N	2.42	0.47
1:B:141:HIS:C	1:B:142:ASN:CG	2.83	0.47
1:A:89:LEU:O	1:A:93:VAL:HG23	2.15	0.46
1:B:459:SER:OG	1:B:460:PRO:HD3	2.16	0.46
1:B:303:ARG:NH2	4:B:894:HOH:O	2.48	0.46
1:B:237:LEU:O	1:B:241:ILE:HG13	2.15	0.46
1:A:87:ALA:O	1:A:91:VAL:HG23	2.15	0.46
1:A:524:SER:OG	1:A:527:GLU:HG3	2.15	0.45
1:B:309:LYS:C	1:B:310:LEU:HD12	2.42	0.45
1:A:412:LEU:HD23	1:B:375:THR:HB	1.97	0.45
1:A:374:ASP:HB2	4:A:887:HOH:O	2.17	0.45
1:A:459:SER:OG	1:A:460:PRO:HD3	2.16	0.45
1:A:162:GLN:HG3	1:A:203:LEU:HD21	1.99	0.44
1:A:276:PHE:CE1	1:A:280:LYS:HD2	2.52	0.44
1:A:505:LEU:HD11	1:A:515:GLN:CD	2.42	0.44
1:A:280:LYS:HE3	1:A:597:TYR:CD2	2.53	0.44
1:B:510:VAL:HG23	4:B:959:HOH:O	2.17	0.44
1:B:492:LEU:HD12	1:B:492:LEU:C	2.43	0.44
1:A:359:THR:OG1	1:A:362:GLU:HG3	2.17	0.44
1:A:561:ALA:O	1:A:564:ILE:HG22	2.17	0.43
1:A:237:LEU:O	1:A:241:ILE:HG13	2.19	0.43
1:B:405:LYS:HD2	1:B:405:LYS:C	2.43	0.43
1:B:458:ILE:HG21	1:B:485:LEU:HD22	2.00	0.43
1:A:169:GLN:OE1	1:A:210:THR:HB	2.18	0.43
1:A:477:SER:O	1:A:480:GLN:HG2	2.19	0.43
1:A:577:GLY:O	1:A:582:HIS:HA	2.18	0.43
1:B:162:GLN:HG3	1:B:203:LEU:HD21	2.00	0.43
1:B:565:GLY:O	1:B:569:GLN:HG3	2.18	0.43
1:B:139:CYS:HB2	1:B:146:GLU:HB2	2.01	0.42
1:B:561:ALA:O	1:B:564:ILE:HG22	2.19	0.42
1:A:233:ILE:HG22	1:A:234:ASP:H	1.84	0.42
1:A:565:GLY:O	1:A:569:GLN:HG3	2.20	0.42
1:B:482:HIS:CE1	1:B:484:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:MET:HG2	1:B:272:ASN:N	2.34	0.42
1:A:405:LYS:HD2	1:A:405:LYS:C	2.45	0.42
1:B:480:GLN:O	1:B:481:TYR:HB2	2.20	0.42
1:A:171:VAL:O	1:A:171:VAL:HG12	2.20	0.42
1:B:101:MET:HG2	1:B:105:GLN:HB2	2.01	0.41
1:B:245:LEU:HD23	1:B:245:LEU:HA	1.89	0.41
1:B:232:GLU:C	1:B:233:ILE:HG13	2.45	0.41
1:A:175:PHE:CD1	1:A:175:PHE:N	2.88	0.41
1:A:151:TYR:CD1	1:A:192:LYS:HG2	2.56	0.41
1:B:175:PHE:CD1	1:B:175:PHE:N	2.88	0.41
1:B:80:GLU:O	1:B:81:ARG:C	2.64	0.41
1:B:151:TYR:CD1	1:B:192:LYS:HG2	2.56	0.41
1:B:171:VAL:O	1:B:171:VAL:HG12	2.21	0.41
1:A:162:GLN:CG	1:A:203:LEU:HD21	2.51	0.41
1:B:85:ARG:HH21	1:B:277:GLU:HG2	1.86	0.41
1:B:149:ASP:O	1:B:150:LEU:C	2.64	0.40
1:B:122:PHE:O	1:B:126:ILE:HG13	2.21	0.40
1:A:515:GLN:CD	1:A:515:GLN:N	2.78	0.40
1:B:367:THR:O	1:B:371:LYS:HG3	2.22	0.40
1:B:359:THR:OG1	1:B:362:GLU:HG3	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	528/549 (96%)	507 (96%)	17 (3%)	4 (1%)	16	20
1	B	519/549 (94%)	489 (94%)	26 (5%)	4 (1%)	16	20
All	All	1047/1098 (95%)	996 (95%)	43 (4%)	8 (1%)	16	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	TYR
1	A	77	TYR
1	A	177	ASN
1	B	136	GLU
1	B	142	ASN
1	B	481	TYR
1	A	225	LYS
1	B	77	TYR

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	468/480 (98%)	463 (99%)	5 (1%)	65	81
1	B	463/480 (96%)	456 (98%)	7 (2%)	57	75
All	All	931/960 (97%)	919 (99%)	12 (1%)	61	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	A	209	ASP
1	A	485	LEU
1	A	492	LEU
1	A	571	ILE
1	B	209	ASP
1	B	271	MET
1	B	304	LEU
1	B	485	LEU
1	B	492	LEU
1	B	498	LEU
1	B	571	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	173	ASN
1	A	223	GLN
1	A	254	GLN
1	A	282	ASN
1	A	531	HIS
1	B	82	HIS
1	B	92	GLN
1	B	135	ASN
1	B	162	GLN
1	B	163	HIS
1	B	169	GLN
1	B	173	ASN
1	B	254	GLN
1	B	282	ASN
1	B	531	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BP2	A	801	2	19,20,20	1.25	2 (10%)	32,35,35	1.76	5 (15%)
3	BP2	B	802	2	19,20,20	1.30	2 (10%)	32,35,35	1.74	6 (18%)

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	BP2	A	801	2	-	2/11/42/42	0/3/2/2
3	BP2	B	802	2	-	3/11/42/42	0/3/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	BP2	P2-O4	3.32	1.60	1.50
3	B	802	BP2	P2-O4	3.03	1.59	1.50
3	B	802	BP2	P1-O3	-2.20	1.52	1.59
3	A	801	BP2	P1-O1	2.01	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	BP2	C4-C5-C8	4.92	108.57	102.53
3	B	802	BP2	C4-C5-C8	4.84	108.47	102.53
3	A	801	BP2	C8-C2-C3	4.51	106.43	100.64
3	B	802	BP2	C8-C2-C3	4.31	106.18	100.64
3	B	802	BP2	C2-C8-C5	-2.77	88.06	93.67
3	A	801	BP2	C2-C8-C5	-2.72	88.17	93.67
3	A	801	BP2	O3-C3-C2	2.34	113.22	110.03
3	B	802	BP2	O3-C3-C2	2.34	113.21	110.03
3	A	801	BP2	C6-C7-C2	-2.12	100.44	104.23
3	B	802	BP2	C7-C2-C8	2.06	104.84	101.56
3	B	802	BP2	C6-C7-C2	-2.04	100.57	104.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	BP2	C3-O3-P1-O1

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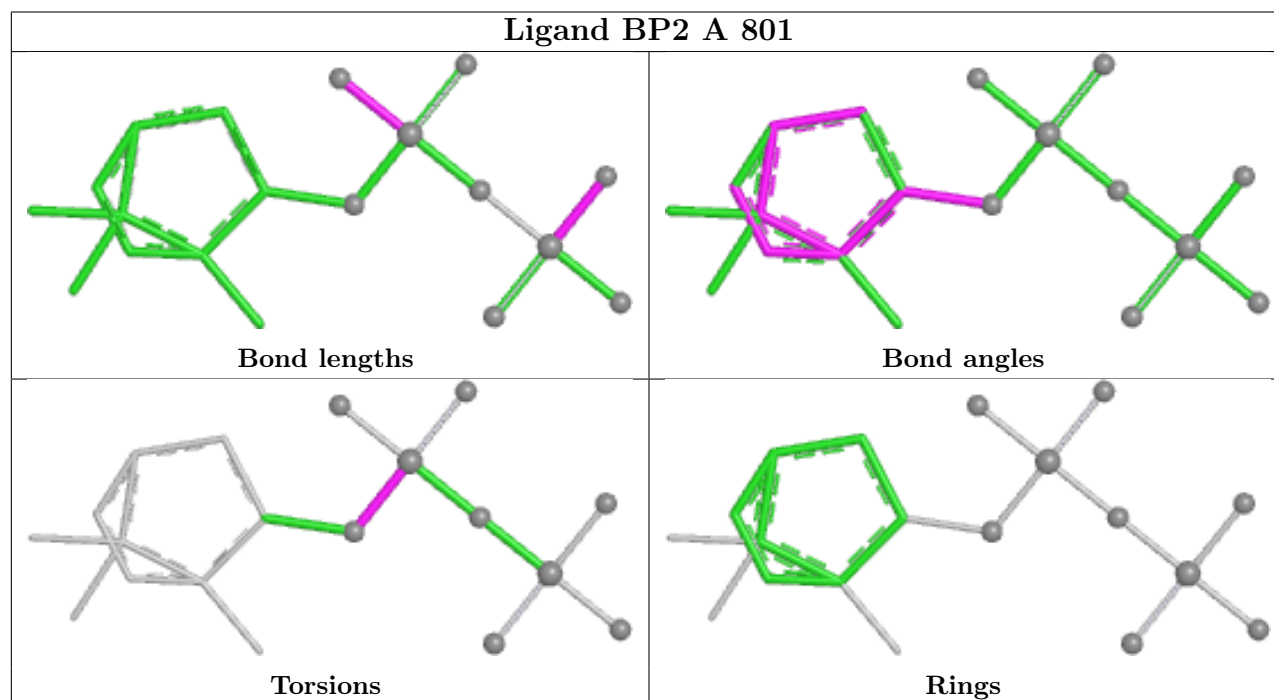
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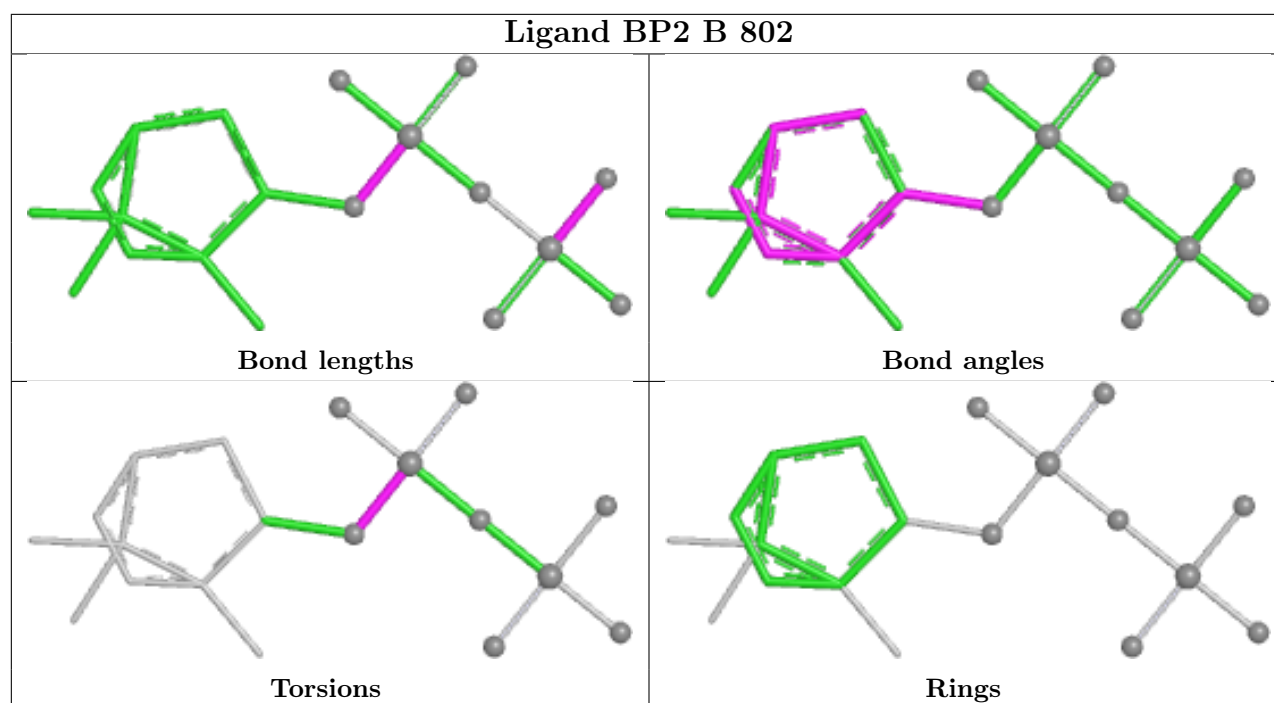
Mol	Chain	Res	Type	Atoms
3	A	801	BP2	C3-O3-P1-O
3	B	802	BP2	C3-O3-P1-O1
3	B	802	BP2	C3-O3-P1-O
3	B	802	BP2	C3-O3-P1-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	534/549 (97%)	0.27	34 (6%) 25 27	21, 38, 71, 93	0
1	B	527/549 (95%)	0.45	44 (8%) 17 19	20, 41, 89, 114	0
All	All	1061/1098 (96%)	0.36	78 (7%) 20 22	20, 40, 81, 114	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	LEU	6.4
1	B	506	ALA	6.3
1	B	578	PHE	5.5
1	B	577	GLY	4.8
1	A	78	THR	4.3
1	A	54	ILE	4.3
1	B	145	VAL	4.2
1	B	148	MET	4.1
1	B	228	GLU	4.0
1	B	142	ASN	4.0
1	B	143	ASN	3.9
1	B	510	VAL	3.8
1	B	140	PHE	3.8
1	A	579	GLY	3.8
1	B	274	LEU	3.5
1	B	141	HIS	3.5
1	B	62	PRO	3.5
1	A	233	ILE	3.5
1	B	146	GLU	3.5
1	A	598	ALA	3.4
1	A	137	HIS	3.4
1	B	85	ARG	3.4
1	B	507	ARG	3.4
1	B	225	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	3.3
1	A	140	PHE	3.2
1	B	172	PHE	3.1
1	B	147	LYS	3.1
1	A	221	CYS	3.1
1	B	96	LEU	3.0
1	B	583	SER	3.0
1	A	234	ASP	3.0
1	B	233	ILE	2.9
1	B	586	TYR	2.9
1	B	231	ASN	2.9
1	A	174	CYS	2.8
1	B	234	ASP	2.8
1	A	141	HIS	2.8
1	B	64	LEU	2.7
1	B	174	CYS	2.7
1	B	222	LEU	2.7
1	A	167	ILE	2.7
1	A	442	ASP	2.6
1	A	582	HIS	2.6
1	B	63	ALA	2.6
1	A	580	VAL	2.6
1	B	139	CYS	2.6
1	B	183	PHE	2.6
1	B	138	LYS	2.5
1	A	181	ILE	2.5
1	A	175	PHE	2.5
1	A	505	LEU	2.5
1	A	183	PHE	2.4
1	A	171	VAL	2.4
1	B	226	LEU	2.4
1	A	81	ARG	2.4
1	A	597	TYR	2.4
1	A	227	ASP	2.4
1	B	571	ILE	2.4
1	A	172	PHE	2.3
1	B	500	THR	2.3
1	A	577	GLY	2.3
1	B	137	HIS	2.2
1	B	224	LYS	2.2
1	A	179	LYS	2.2
1	B	237	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	576	ASP	2.2
1	A	77	TYR	2.2
1	A	235	GLU	2.2
1	B	144	GLU	2.2
1	A	506	ALA	2.2
1	A	187	LEU	2.1
1	A	585	THR	2.1
1	B	100	LYS	2.1
1	A	218	ALA	2.0
1	A	232	GLU	2.0
1	A	180	GLY	2.0
1	B	78	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

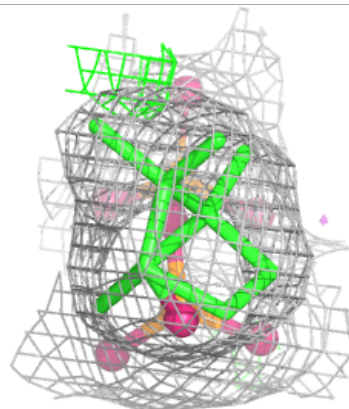
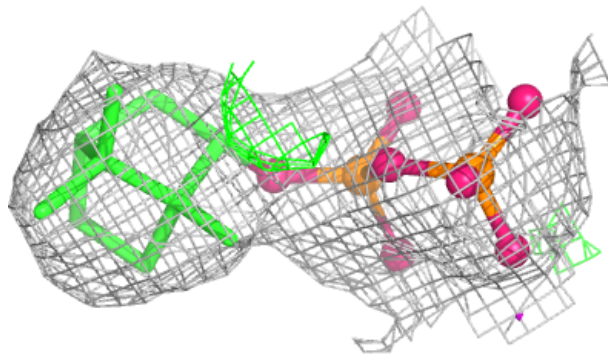
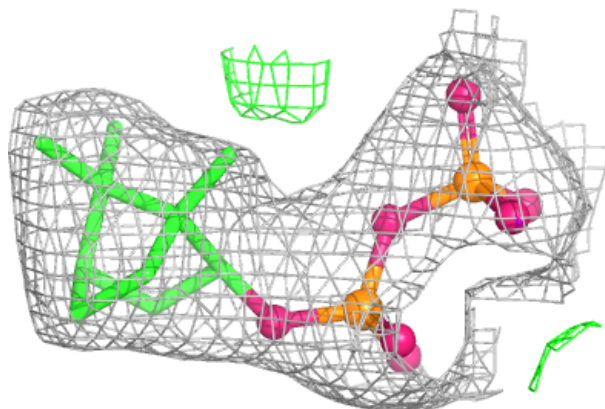
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	706	1/1	0.89	0.08	45,45,45,45	0
3	BP2	B	802	19/19	0.97	0.08	36,44,49,49	0
3	BP2	A	801	19/19	0.98	0.06	26,33,35,37	0
2	MG	B	704	1/1	0.99	0.05	25,25,25,25	0
2	MG	B	705	1/1	0.99	0.02	38,38,38,38	0
2	MG	A	701	1/1	0.99	0.02	29,29,29,29	0
2	MG	A	702	1/1	0.99	0.03	28,28,28,28	0
2	MG	A	703	1/1	0.99	0.03	37,37,37,37	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.

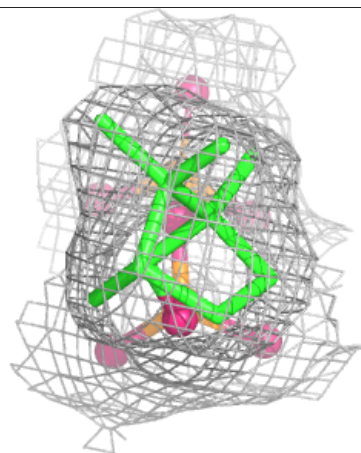
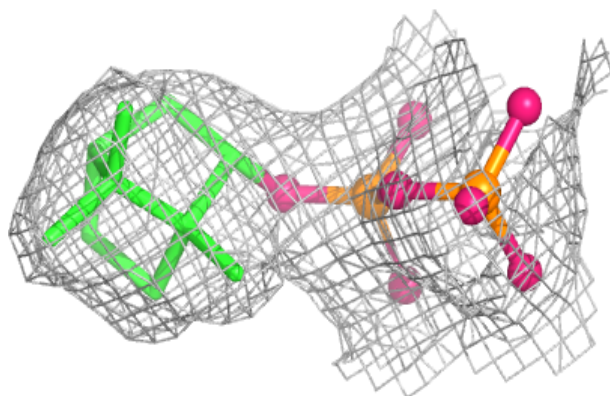
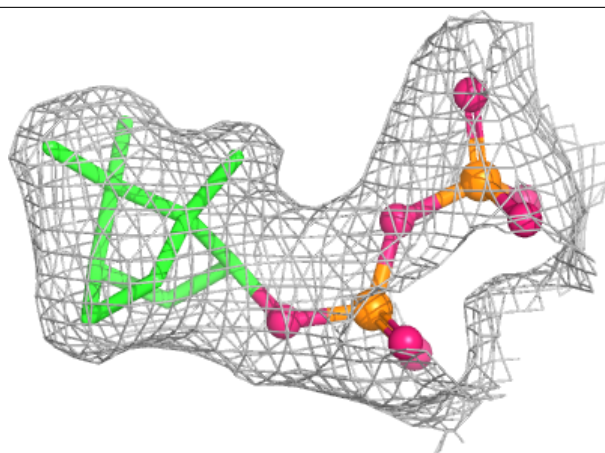
Electron density around BP2 B 802:

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



Electron density around BP2 A 801:

$2mF_o-DF_c$ (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.