



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 1N24
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

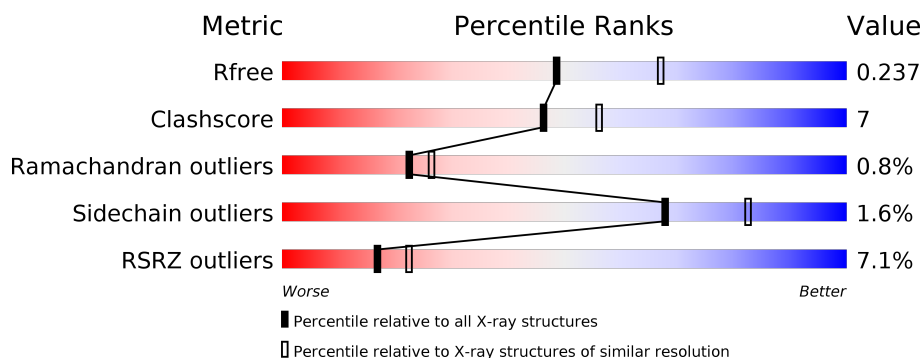
1 Overall quality at a glance

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div>82%</div> <div>14%</div> <div>••</div> </div>
1	B	549	<div> <div>8%</div> <div>79%</div> <div>17%</div> <div>••</div> </div>

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.

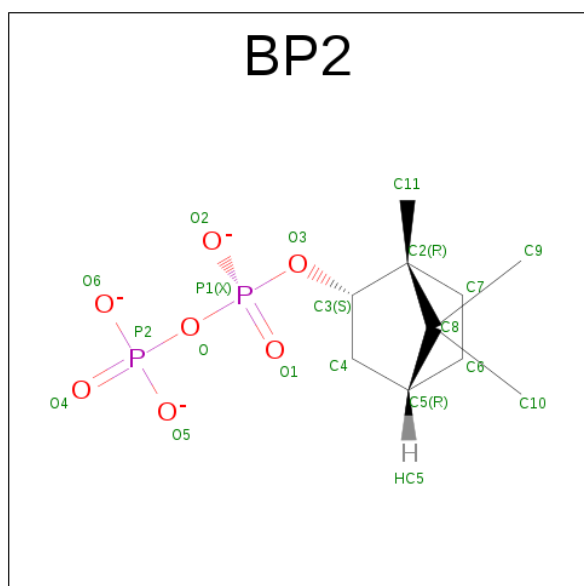
- Molecule 1 is a protein called (+)-bornyl diphosphate synthase.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is (+)-BORNYL DIPHOSPHATE (three-letter code: 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		

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) 94.8 (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 1.0	Depositor
R, R_{free}	0.210 , 0.238 0.210 , 0.237	Depositor DCC
R_{free} test set	2465 reflections (4.03%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	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	0.41	1/4527 (0.0%)	0.58	3/6135 (0.0%)
1	B	0.38	0/4460	0.54	1/6042 (0.0%)
All	All	0.40	1/8987 (0.0%)	0.56	4/12177 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PRO	CA-C	-8.17	1.36	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PRO	CA-N-CD	-10.30	97.08	111.50
1	A	76	PRO	CB-CA-C	-5.25	98.88	112.00
1	B	480	GLN	N-CA-C	-5.17	97.05	111.00
1	A	76	PRO	O-C-N	-5.07	114.58	122.70

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	62	0
1	B	4346	0	4236	65	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	19	0	17	0	0
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	125	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 7.

All (125) 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:141:HIS:O	1:B:142:ASN:OD1	1.86	0.93
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:HIS:O	1:B:142:ASN:CG	2.33	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: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:479:TYR:C	1:B:481:TYR:H	1.96	0.63
1:B:479:TYR:C	1:B:481:TYR:N	2.43	0.63
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:O	1:B:492:LEU:HD12	1.99	0.61
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:A:224:LYS:C	1:A:226:LEU:H	2.05	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:452:VAL:HG22	1:B:492:LEU:HG	1.86	0.56
1:B:81:ARG:NH1	1:B:82:HIS:CE1	2.72	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:B:500:THR:HG22	1:B:576:ASP:HB2	1.88	0.55
1:A:101:MET:CE	1:A:105:GLN:HB3	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:479:TYR:C	1:A:481:TYR:N	2.54	0.51
1:B:148:MET:CE	1:B:174:CYS:HB3	2.41	0.50
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:515:GLN:H	1:A:515:GLN:CD	2.15	0.50
1:A:570:PHE:HB2	4:A:858:HOH:O	2.11	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
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:101:MET:HE1	1:A:105:GLN:HB3	1.96	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:A:224:LYS:C	1:A:226:LEU:N	2.68	0.47
1:B:125:GLU:OE1	1:B:125:GLU:N	2.42	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:101:MET:HE2	1:A:105:GLN:HB3	1.98	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:233:ILE:O	1:B:234:ASP:C	2.53	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:O	1:A:241:ILE:HG13	2.19	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:B:148:MET:HE2	1:B:174:CYS:HB3	2.00	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:171:VAL:O	1:A:171:VAL:HG12	2.20	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
1:B:271:MET:HG2	1:B:272:ASN:N	2.34	0.42
1:B:480:GLN:O	1:B:481:TYR:HB2	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:A:175:PHE:N	1:A:175:PHE:CD1	2.88	0.41
1:A:151:TYR:CD1	1:A:192:LYS:HG2	2.56	0.41
1:B:171:VAL:HG12	1:B:171:VAL:O	2.21	0.41
1:B:175:PHE:CD1	1:B:175:PHE:N	2.88	0.41
1:B:151:TYR:CD1	1:B:192:LYS:HG2	2.56	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:122:PHE:O	1:B:126:ILE:HG13	2.21	0.40
1:B:309:LYS:C	1:B:310:LEU:HD12	2.42	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	22	26
1	B	519/549 (94%)	489 (94%)	26 (5%)	4 (1%)	22	26
All	All	1047/1098 (95%)	996 (95%)	43 (4%)	8 (1%)	22	26

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%)	460 (98%)	8 (2%)	66	81
1	B	463/480 (96%)	456 (98%)	7 (2%)	70	83
All	All	931/960 (97%)	916 (98%)	15 (2%)	68	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	A	182	ASP
1	A	209	ASP
1	A	254	GLN
1	A	485	LEU
1	A	492	LEU
1	A	571	ILE
1	A	582	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	ASP
1	B	209	ASP
1	B	227	ASP
1	B	254	GLN
1	B	323	TRP
1	B	492	LEU
1	B	571	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	254	GLN
1	A	282	ASN
1	A	531	HIS
1	B	82	HIS
1	B	169	GLN
1	B	173	ASN
1	B	254	GLN
1	B	531	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BP2	A	801	2	19,20,20	1.26	2 (10%)	27,35,35	2.16	6 (22%)
3	BP2	B	802	2	19,20,20	1.33	2 (10%)	27,35,35	2.23	6 (22%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	BP2	P1-O3	-3.26	1.52	1.60
3	A	801	BP2	P1-O3	-2.98	1.53	1.60
3	B	802	BP2	P2-O4	2.69	1.59	1.50
3	A	801	BP2	P2-O4	2.95	1.60	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	BP2	C2-C8-C5	-2.61	88.06	93.78
3	A	801	BP2	C2-C8-C5	-2.56	88.17	93.78
3	A	801	BP2	C6-C7-C2	-2.17	100.44	104.22
3	B	802	BP2	C6-C7-C2	-2.09	100.57	104.22
3	A	801	BP2	C7-C2-C8	2.28	104.72	101.48
3	B	802	BP2	C7-C2-C8	2.37	104.84	101.48
3	B	802	BP2	C8-C2-C3	4.16	106.18	100.64
3	A	801	BP2	C8-C2-C3	4.35	106.43	100.64
3	B	802	BP2	C4-C5-C8	4.96	108.47	102.56
3	A	801	BP2	C4-C5-C8	5.04	108.57	102.56
3	A	801	BP2	O-P1-O3	6.08	112.91	102.05
3	B	802	BP2	O-P1-O3	6.87	114.33	102.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	33 (6%) 21 28	21, 38, 71, 93	0
1	B	527/549 (95%)	0.31	42 (7%) 13 17	20, 41, 89, 114	0
All	All	1061/1098 (96%)	0.24	75 (7%) 17 22	20, 40, 81, 114	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	GLU	7.4
1	B	143	ASN	6.8
1	B	147	LYS	6.4
1	B	142	ASN	6.3
1	B	506	ALA	6.3
1	B	148	MET	5.2
1	B	141	HIS	4.7
1	B	505	LEU	4.7
1	B	583	SER	4.7
1	B	145	VAL	4.5
1	B	238	LEU	4.3
1	A	233	ILE	4.2
1	A	181	ILE	4.0
1	B	233	ILE	4.0
1	B	584	LYS	3.8
1	A	178	GLU	3.8
1	B	235	GLU	3.7
1	A	138	LYS	3.7
1	A	598	ALA	3.6
1	B	226	LEU	3.6
1	A	54	ILE	3.5
1	A	344	ILE	3.5
1	A	78	THR	3.5
1	A	137	HIS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	GLU	3.4
1	A	235	GLU	3.4
1	A	343	ILE	3.4
1	B	586	TYR	3.3
1	B	189	GLN	3.3
1	B	178	GLU	3.2
1	B	574	HIS	3.1
1	B	578	PHE	3.1
1	A	180	GLY	3.1
1	B	138	LYS	3.1
1	B	100	LYS	3.0
1	B	225	LYS	2.9
1	B	232	GLU	2.9
1	A	189	GLN	2.9
1	A	179	LYS	2.8
1	A	346	LEU	2.8
1	B	224	LYS	2.8
1	B	507	ARG	2.7
1	B	274	LEU	2.7
1	A	453	ALA	2.7
1	B	231	ASN	2.7
1	A	224	LYS	2.7
1	B	242	ARG	2.6
1	B	228	GLU	2.6
1	A	347	ALA	2.6
1	B	180	GLY	2.6
1	B	587	GLU	2.5
1	B	62	PRO	2.5
1	B	577	GLY	2.5
1	A	234	ASP	2.5
1	B	177	ASN	2.4
1	A	134	TYR	2.4
1	B	140	PHE	2.4
1	A	141	HIS	2.4
1	B	80	GLU	2.3
1	A	350	ILE	2.3
1	A	506	ALA	2.3
1	A	457	ILE	2.3
1	B	227	ASP	2.2
1	B	510	VAL	2.2
1	A	345	VAL	2.1
1	A	522	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	340	ALA	2.1
1	A	140	PHE	2.1
1	A	564	ILE	2.1
1	A	349	VAL	2.1
1	A	61	GLN	2.0
1	A	127	LYS	2.0
1	B	144	GLU	2.0
1	B	234	ASP	2.0
1	B	96	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	BP2	A	801	19/19	0.98	0.17	-0.15	26,33,35,37	0
3	BP2	B	802	19/19	0.97	0.13	-0.55	36,44,49,49	0
2	MG	A	701	1/1	0.98	0.11	-1.11	29,29,29,29	0
2	MG	B	705	1/1	0.97	0.06	-1.13	38,38,38,38	0
2	MG	A	702	1/1	0.97	0.10	-1.36	28,28,28,28	0
2	MG	A	703	1/1	0.97	0.11	-1.48	37,37,37,37	0
2	MG	B	704	1/1	0.96	0.04	-3.99	25,25,25,25	0
2	MG	B	706	1/1	0.73	0.08	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.