



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:20 pm BST

PDB ID : 4R0Q  
Title : Structure of a putative peptidoglycan glycosyltransferase from *Atopobium parvulum* in complex with cephalothin  
Authors : Filippova, E.V.; Minasov, G.; Kiryukhina, O.; Clancy, S.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2014-08-01  
Resolution : 2.00 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

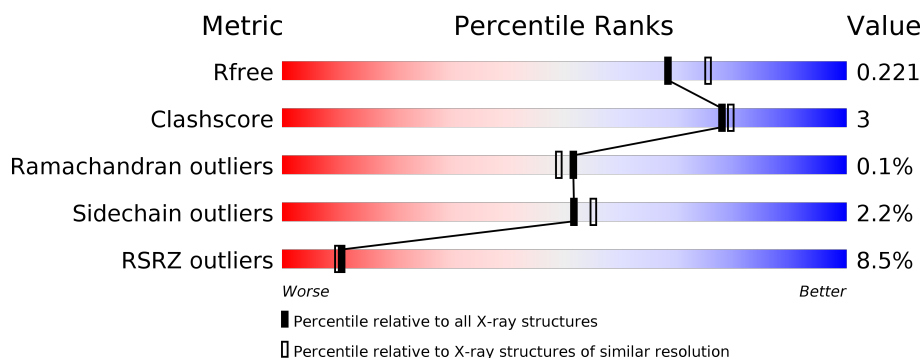
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	482	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>• •</div> <div>14%</div> </div> </div>
1	B	482	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>7% •</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6398 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 Peptidoglycan glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	Se	0	1	0
			2982	1851	508	608	2	13			
1	B	412	Total	C	N	O	S	Se	0	0	0
			2967	1843	503	606	2	13			

There are 64 discrepancies between the modelled and reference sequences:

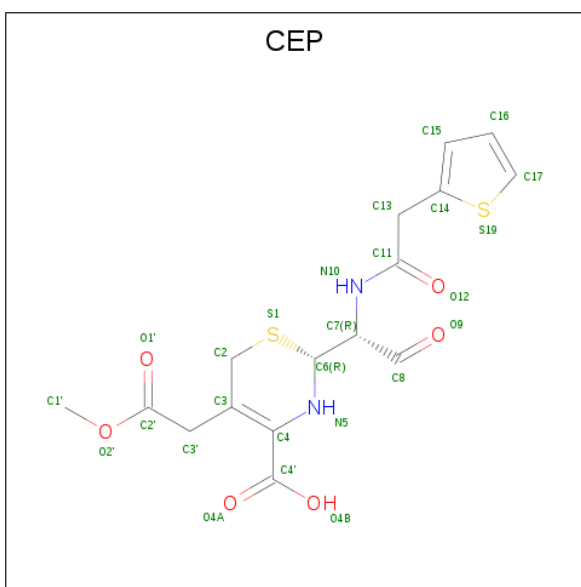
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
A	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	480	SER	-	EXPRESSION TAG	UNP C8W8H7
A	481	SER	-	EXPRESSION TAG	UNP C8W8H7
A	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
A	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
A	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
A	487	SER	-	EXPRESSION TAG	UNP C8W8H7
A	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
A	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
A	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	495	THR	-	EXPRESSION TAG	UNP C8W8H7
A	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	497	ASN	-	EXPRESSION TAG	UNP C8W8H7

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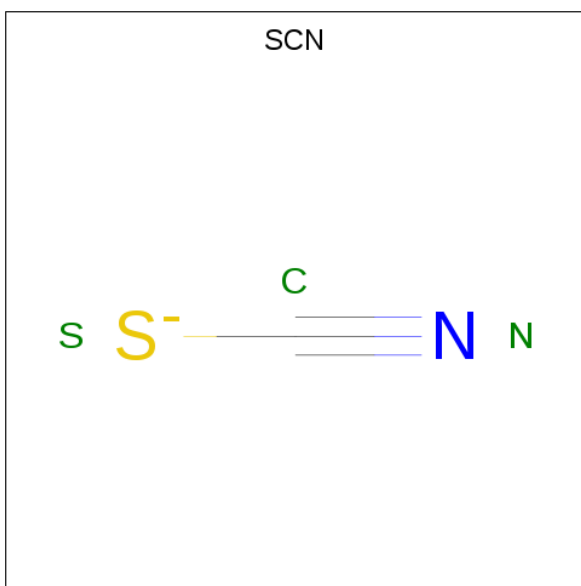
Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
A	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	502	SER	-	EXPRESSION TAG	UNP C8W8H7
A	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
A	504	ALA	-	EXPRESSION TAG	UNP C8W8H7
B	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
B	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	480	SER	-	EXPRESSION TAG	UNP C8W8H7
B	481	SER	-	EXPRESSION TAG	UNP C8W8H7
B	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
B	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
B	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
B	487	SER	-	EXPRESSION TAG	UNP C8W8H7
B	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
B	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
B	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	495	THR	-	EXPRESSION TAG	UNP C8W8H7
B	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	497	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
B	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	502	SER	-	EXPRESSION TAG	UNP C8W8H7
B	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	504	ALA	-	EXPRESSION TAG	UNP C8W8H7

- Molecule 2 is CEPHALOTHIN GROUP (three-letter code: CEP) (formula: C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>6</sub>S<sub>2</sub>).



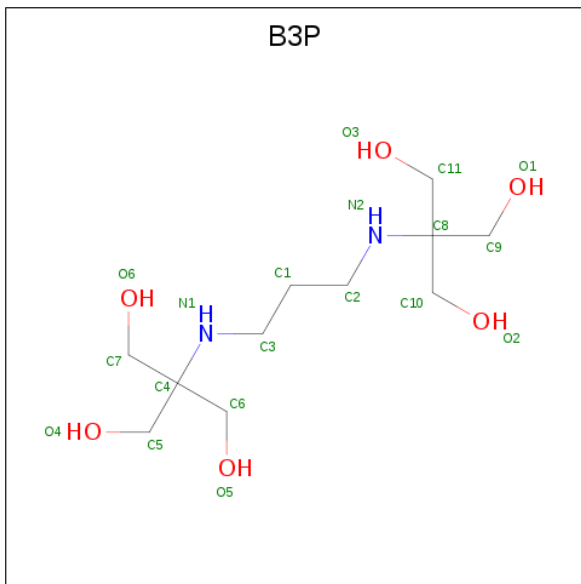
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			27	18	2	4	3		
2	B	1	Total	C	N	O	S	0	0
			22	14	2	4	2		

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	11	2	6		
4	B	1	Total	C	N	O	0	0
			19	11	2	6		

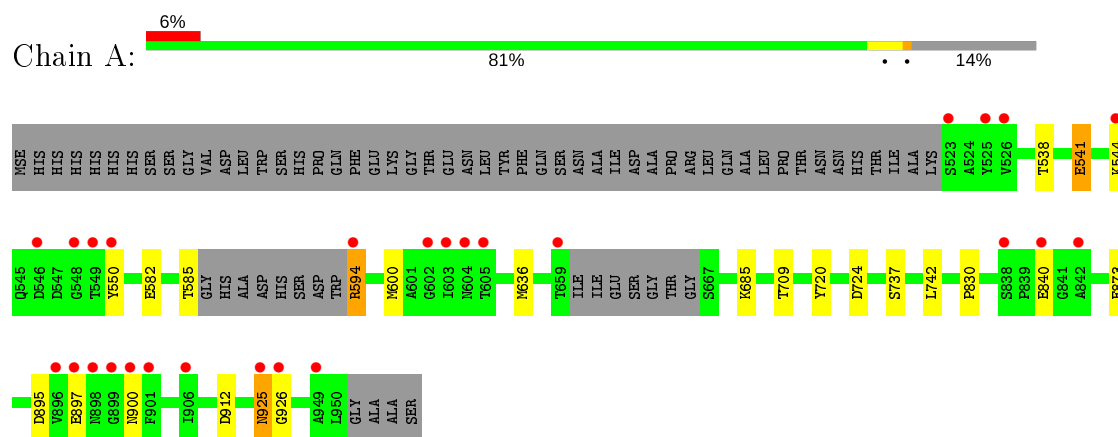
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total	O	0	1
			208	208		
5	B	148	Total	O	0	0
			148	148		

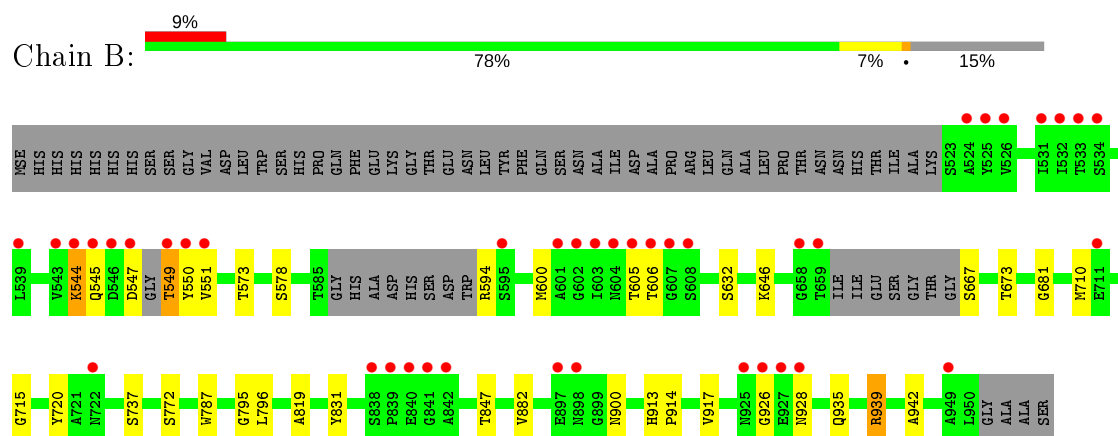
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Peptidoglycan glycosyltransferase



#### • Molecule 1: Peptidoglycan glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.55Å 70.00Å 115.23Å 90.00° 96.76° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.00) 98.6 (29.86-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.179 , 0.217 0.186 , 0.221	Depositor DCC
$R_{free}$ test set	3668 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: SCN, B3P, CEP

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	0.73	0/3019	0.83	2/4096 (0.0%)
1	B	0.69	0/3003	0.81	0/4074
All	All	0.71	0/6022	0.82	2/8170 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	541	GLU	CB-CA-C	-5.16	100.08	110.40

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	2982	0	2911	13	0
1	B	2967	0	2896	21	0
2	A	27	0	10	2	0
2	B	22	0	11	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	26	0	0
5	A	208	0	0	2	0
5	B	148	0	0	3	0
All	All	6398	0	5880	35	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 3.

All (35) 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:594[A]:ARG:HD2	1:A:600:MSE:HE1	1.76	0.66
1:B:882:VAL:HG21	1:B:942:ALA:HB2	1.79	0.65
1:B:900:ASN:OD1	1:B:926:GLY:N	2.32	0.62
1:A:594[A]:ARG:CD	1:A:600:MSE:HE1	2.31	0.60
1:B:545:GLN:OE1	1:B:551:VAL:HG12	2.03	0.58
1:B:573:THR:HB	1:B:578:SER:HB2	1.87	0.57
1:B:796:LEU:HD21	5:B:1107:HOH:O	2.04	0.56
1:A:720:TYR:CE1	2:A:1001[B]:CEP:H16	2.41	0.56
1:A:544:LYS:HB2	1:A:550:TYR:CE1	2.41	0.55
1:B:547:ASP:HB2	1:B:549:THR:OG1	2.08	0.54
2:A:1001[A]:CEP:H17	5:A:1306:HOH:O	2.09	0.52
1:A:538:THR:HG21	1:A:541:GLU:HG3	1.92	0.51
1:B:667:SER:N	5:B:1131:HOH:O	2.45	0.49
1:A:636:MSE:HE2	1:A:830:PRO:HB3	1.95	0.47
1:B:715:GLY:HA3	1:B:787:TRP:CD1	2.50	0.47
1:B:720:TYR:HB2	2:B:1001:CEP:S1	2.55	0.47
1:A:582:GLU:O	1:A:585:THR:HB	2.15	0.46
1:B:681:GLY:O	1:B:795:GLY:HA3	2.16	0.46
1:B:831:TYR:CD2	1:B:847:THR:HG21	2.51	0.45
1:A:912:ASP:HB2	5:A:1274:HOH:O	2.16	0.45
1:B:545:GLN:OE1	1:B:551:VAL:CG1	2.64	0.45
1:A:900:ASN:OD1	1:A:926:GLY:N	2.49	0.45
1:B:913:HIS:N	1:B:914:PRO:HD3	2.32	0.45
1:A:685:LYS:HD3	1:A:742:LEU:HG	1.99	0.44
1:B:605:THR:HG22	1:B:606:THR:N	2.34	0.43
1:B:646:LYS:HE2	1:B:673:THR:OG1	2.19	0.43
1:B:594:ARG:HD2	1:B:594:ARG:HA	1.74	0.42
1:B:544:LYS:HA	1:B:550:TYR:CD1	2.54	0.42
1:B:632:SER:HB2	1:B:673:THR:HG22	2.00	0.42
1:A:900:ASN:OD1	1:A:925:ASN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:ALA:HA	1:B:917:VAL:HG21	2.02	0.41
1:B:935:GLN:O	1:B:939:ARG:HG2	2.20	0.41
1:A:897:GLU:N	1:A:897:GLU:OE1	2.53	0.41
1:B:939:ARG:HD2	5:B:1116:HOH:O	2.21	0.41

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	407/482 (84%)	395 (97%)	11 (3%)	1 (0%)	47	44
1	B	404/482 (84%)	389 (96%)	15 (4%)	0	100	100
All	All	811/964 (84%)	784 (97%)	26 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	925	ASN

### 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	315/356 (88%)	308 (98%)	7 (2%)	52	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	314/356 (88%)	306 (98%)	8 (2%)	47	49
All	All	629/712 (88%)	614 (98%)	15 (2%)	52	51

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

Mol	Chain	Res	Type
1	A	594[A]	ARG
1	A	594[B]	ARG
1	A	709	THR
1	A	737	SER
1	A	840	GLU
1	A	873	GLU
1	A	895	ASP
1	B	544	LYS
1	B	549	THR
1	B	600	MSE
1	B	710	MSE
1	B	737	SER
1	B	772	SER
1	B	928	ASN
1	B	939	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	ASN
1	A	722	ASN
1	A	943	GLN
1	B	722	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

7 ligands are modelled in this entry.

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
2	CEP	A	1001[B]	-	17,23,27	2.12	4 (23%)	15,31,36	3.13	7 (46%)
4	B3P	B	1003	-	18,18,18	0.57	0	21,23,23	1.97	2 (9%)
4	B3P	A	1003	-	18,18,18	0.56	0	21,23,23	2.19	4 (19%)
3	SCN	B	1002	-	1,2,2	0.25	0	0,1,1	0.00	-
3	SCN	A	1002	-	1,2,2	0.06	0	0,1,1	0.00	-
2	CEP	B	1001	1	17,23,27	1.38	2 (11%)	15,31,36	2.13	6 (40%)
2	CEP	A	1001[A]	-	17,23,27	2.67	4 (23%)	15,31,36	3.34	8 (53%)

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
2	CEP	A	1001[B]	-	-	2/6/31/37	0/1/2/2
2	CEP	B	1001	1	-	2/6/31/37	0/1/2/2
4	B3P	B	1003	-	-	9/28/28/28	-
4	B3P	A	1003	-	-	12/28/28/28	-
2	CEP	A	1001[A]	-	-	0/6/31/37	0/1/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[A]	CEP	C13-C14	8.45	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[B]	CEP	C13-C14	5.48	1.55	1.51
2	B	1001	CEP	C4'-C4	-4.15	1.45	1.52
2	A	1001[B]	CEP	C4'-C4	-4.02	1.46	1.52
2	A	1001[A]	CEP	C4'-C4	-4.02	1.46	1.52
2	A	1001[B]	CEP	C3-C4	-3.66	1.29	1.34
2	A	1001[A]	CEP	C3-C4	-3.66	1.29	1.34
2	B	1001	CEP	C2-S1	-2.44	1.76	1.82
2	A	1001[B]	CEP	C2-S1	-2.23	1.77	1.82
2	A	1001[A]	CEP	C2-S1	-2.23	1.77	1.82

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	B3P	C2-N2-C8	7.51	126.73	116.08
4	B	1003	B3P	C3-N1-C4	6.24	124.94	116.08
2	A	1001[B]	CEP	C3'-C3-C2	6.11	123.15	113.23
2	A	1001[A]	CEP	C3'-C3-C2	6.11	123.15	113.23
2	A	1001[B]	CEP	C6-N5-C4	5.57	131.42	118.32
2	A	1001[A]	CEP	C6-N5-C4	5.57	131.42	118.32
2	A	1001[B]	CEP	C2-C3-C4	-5.41	114.57	123.48
2	A	1001[A]	CEP	C2-C3-C4	-5.41	114.57	123.48
4	B	1003	B3P	C2-N2-C8	5.29	123.58	116.08
4	A	1003	B3P	C3-N1-C4	5.10	123.32	116.08
2	B	1001	CEP	C6-N5-C4	4.43	128.74	118.32
2	A	1001[A]	CEP	C14-C13-C11	4.15	121.65	113.39
2	A	1001[B]	CEP	O12-C11-N10	-3.73	116.66	122.95
2	A	1001[A]	CEP	O12-C11-N10	-3.73	116.66	122.95
2	A	1001[B]	CEP	C13-C11-N10	3.38	121.33	115.88
2	A	1001[A]	CEP	C13-C11-N10	3.38	121.33	115.88
2	A	1001[B]	CEP	C3-C2-S1	-3.34	112.24	116.98
2	A	1001[A]	CEP	C3-C2-S1	-3.34	112.24	116.98
2	B	1001	CEP	C2-S1-C6	3.15	100.64	94.47
2	A	1001[B]	CEP	C6-C7-N10	2.93	116.36	109.98
2	A	1001[A]	CEP	C6-C7-N10	2.93	116.36	109.98
2	B	1001	CEP	C3'-C3-C4	-2.91	119.91	123.53
2	B	1001	CEP	C13-C11-N10	2.55	119.99	115.88
2	B	1001	CEP	C3'-C3-C2	2.44	117.19	113.23
4	A	1003	B3P	C11-C8-C9	-2.23	105.34	110.04
2	B	1001	CEP	O9-C8-C7	-2.18	118.75	124.83
4	A	1003	B3P	O4-C5-C4	-2.14	107.29	111.63

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	B3P	C5-C4-N1-C3
4	B	1003	B3P	C7-C4-N1-C3
4	B	1003	B3P	N1-C4-C6-O5
4	B	1003	B3P	C5-C4-C6-O5
4	B	1003	B3P	C7-C4-C6-O5
4	A	1003	B3P	C5-C4-N1-C3
4	A	1003	B3P	C6-C4-N1-C3
4	A	1003	B3P	C7-C4-N1-C3
4	A	1003	B3P	N1-C4-C7-O6
4	A	1003	B3P	C5-C4-C7-O6
4	A	1003	B3P	C9-C8-N2-C2
4	A	1003	B3P	C10-C8-N2-C2
4	A	1003	B3P	C11-C8-N2-C2
4	A	1003	B3P	C3-C1-C2-N2
4	B	1003	B3P	C3-C1-C2-N2
4	B	1003	B3P	C1-C3-N1-C4
4	A	1003	B3P	C2-C1-C3-N1
2	B	1001	CEP	O12-C11-C13-C14
4	B	1003	B3P	C6-C4-N1-C3
4	A	1003	B3P	C6-C4-C7-O6
4	A	1003	B3P	C1-C2-N2-C8
2	B	1001	CEP	N10-C11-C13-C14
2	A	1001[B]	CEP	O12-C11-C13-C14
2	A	1001[B]	CEP	N10-C11-C13-C14
4	B	1003	B3P	C2-C1-C3-N1

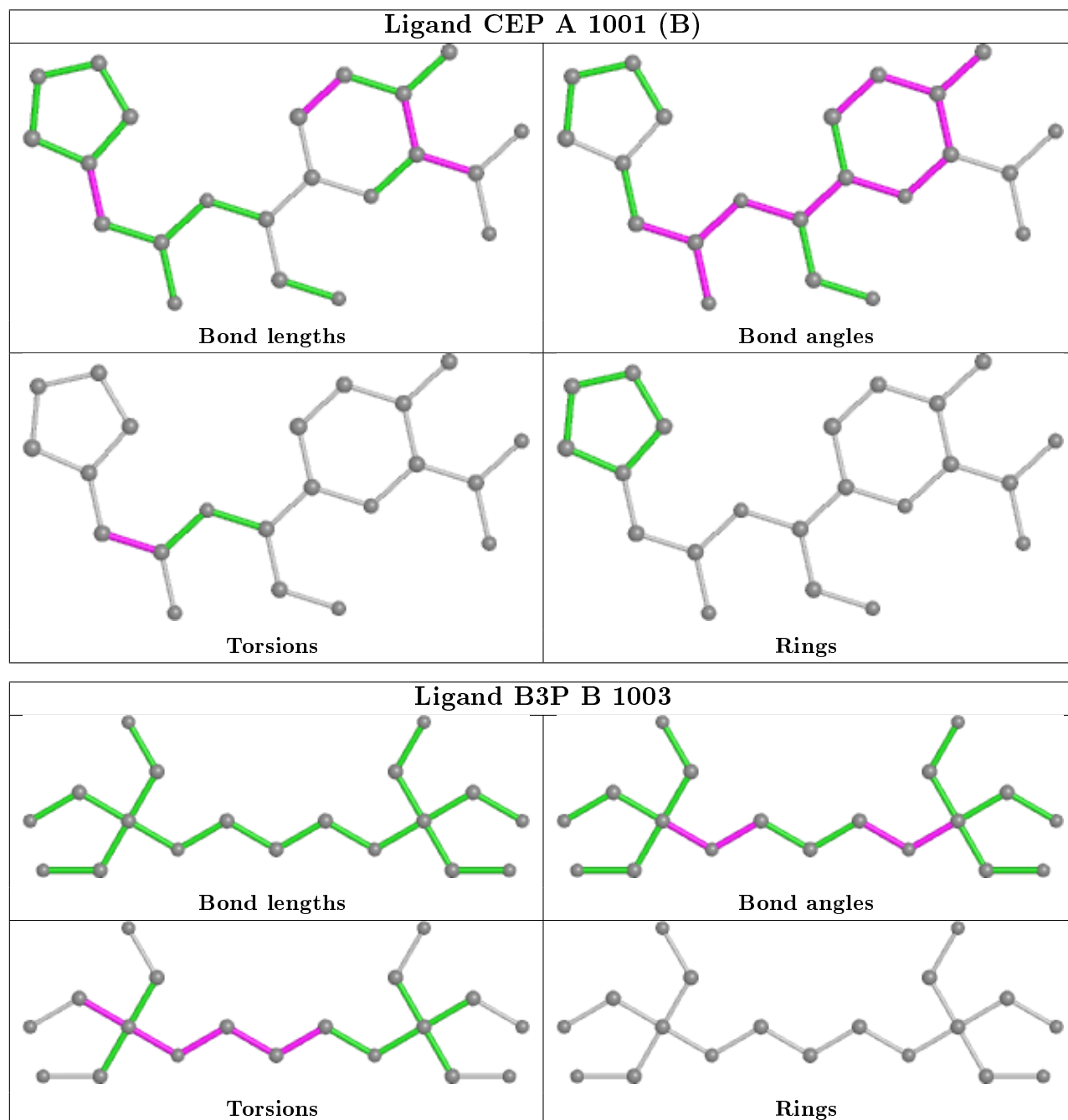
There are no ring outliers.

3 monomers are involved in 3 short contacts:

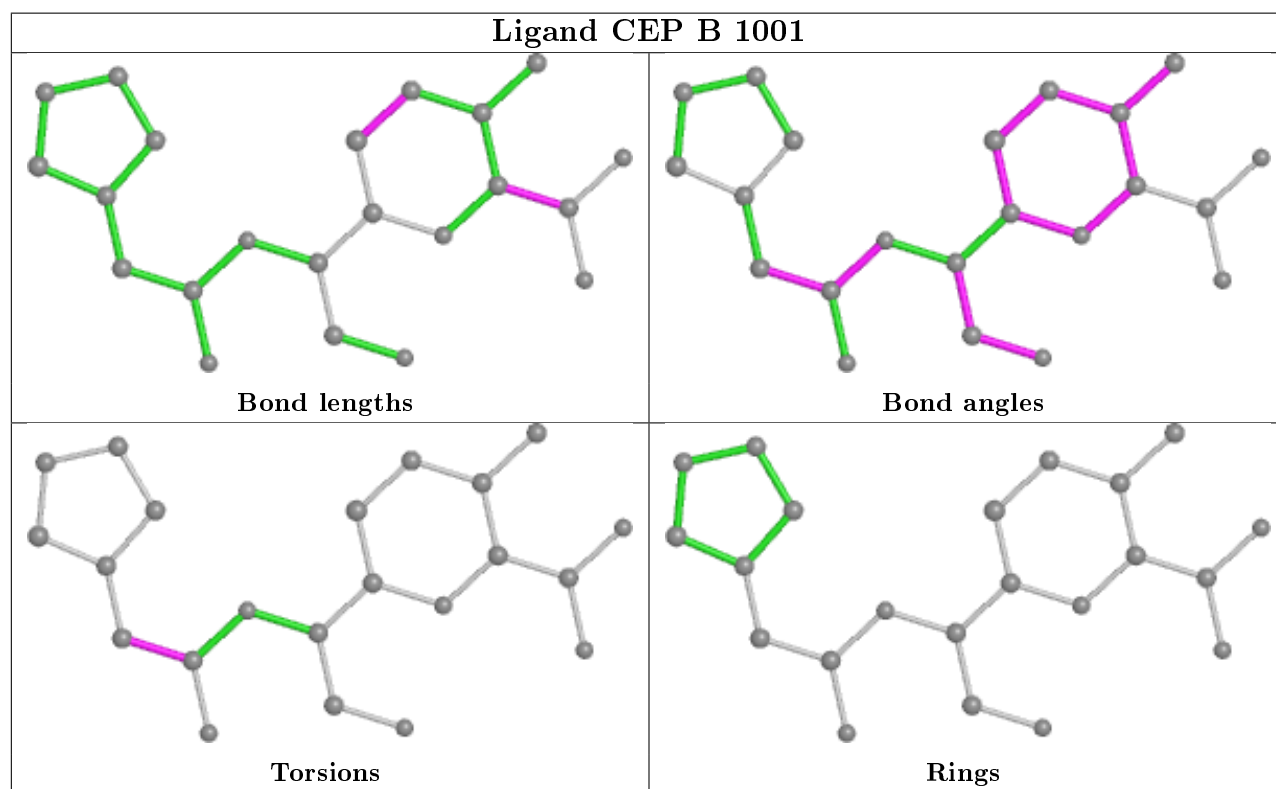
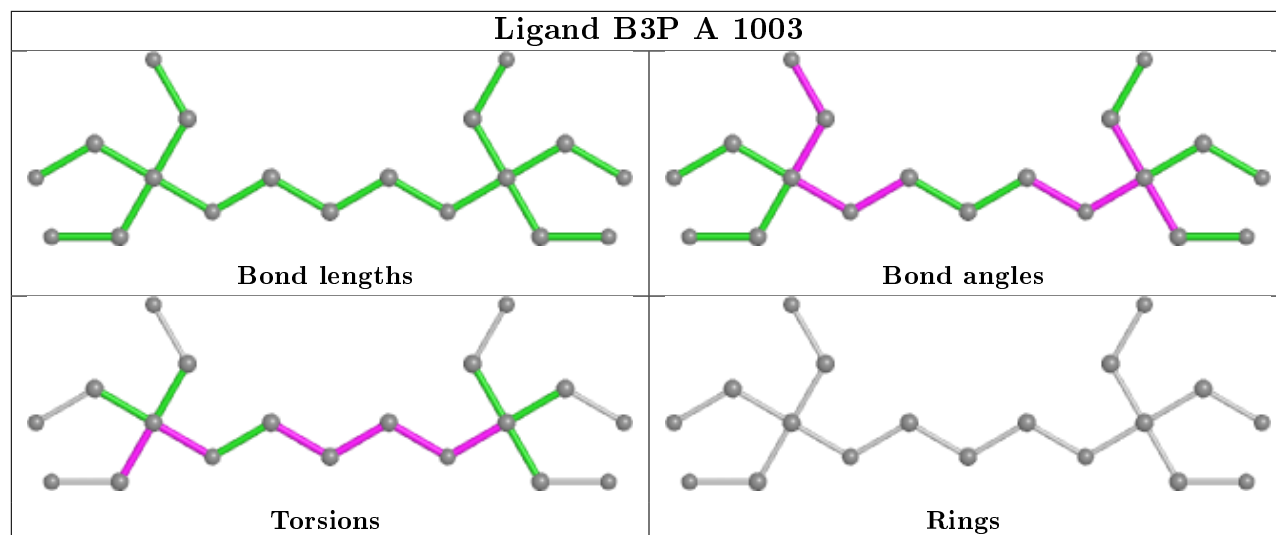
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001[B]	CEP	1	0
2	B	1001	CEP	1	0
2	A	1001[A]	CEP	1	0

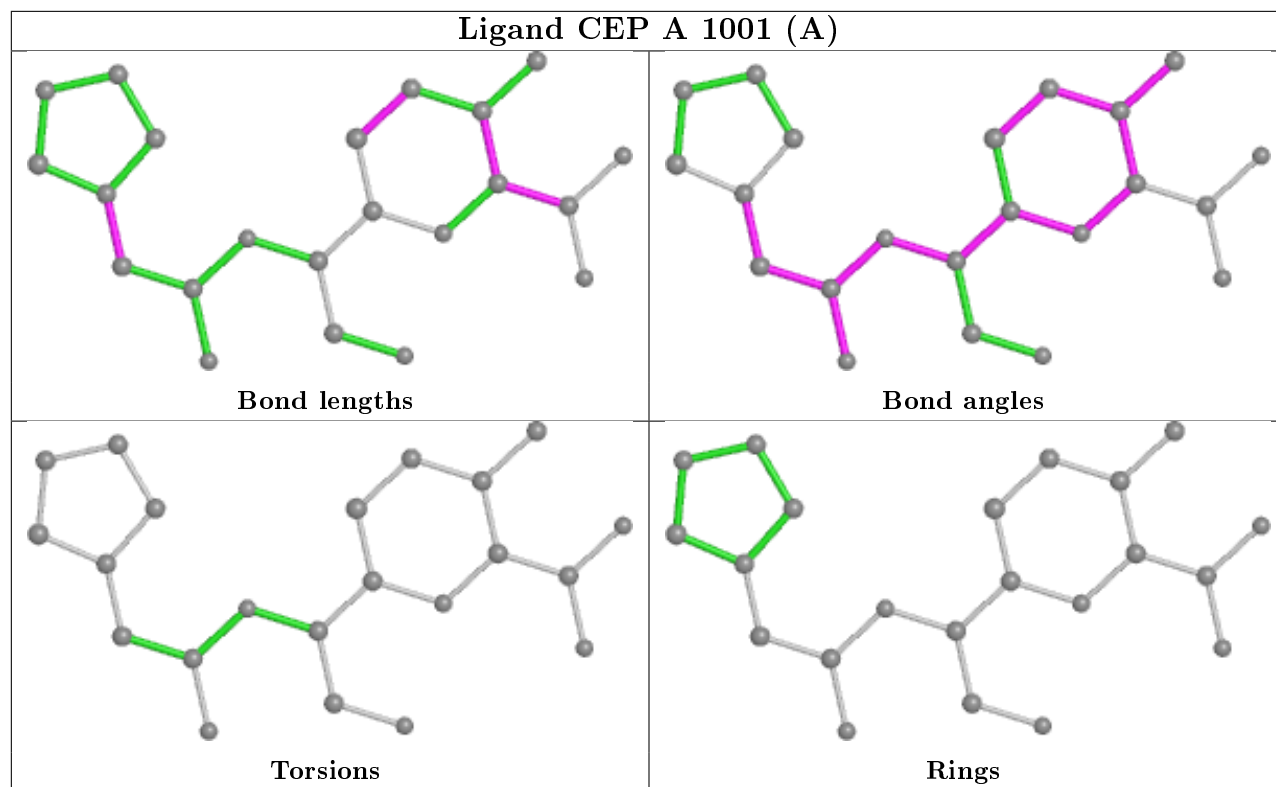
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	400/482 (82%)	-0.01	27 (6%) 17 16	23, 36, 77, 106	0
1	B	399/482 (82%)	0.26	41 (10%) 6 6	25, 41, 107, 127	0
All	All	799/964 (82%)	0.12	68 (8%) 10 10	23, 38, 100, 127	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	ASN	6.2
1	B	549	THR	6.0
1	A	603	ILE	5.8
1	B	842	ALA	5.4
1	B	526	VAL	5.2
1	B	841	GLY	5.1
1	B	543	VAL	4.8
1	B	840	GLU	4.8
1	B	603	ILE	4.8
1	A	549	THR	4.6
1	A	604	ASN	4.6
1	B	604	ASN	4.5
1	B	544	LYS	4.5
1	A	523	SER	4.3
1	B	658	GLY	4.3
1	A	897	GLU	4.0
1	A	602	GLY	4.0
1	A	526	VAL	3.9
1	B	607	GLY	3.9
1	B	606	THR	3.8
1	B	525	TYR	3.7
1	B	602	GLY	3.7
1	A	548	GLY	3.6
1	B	926	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	525	TYR	3.5
1	B	605	THR	3.5
1	A	899	GLY	3.4
1	B	898	ASN	3.4
1	B	539	LEU	3.3
1	B	927	GLU	3.2
1	B	608	SER	3.2
1	B	533	THR	3.2
1	B	897	GLU	3.1
1	B	534	SER	3.1
1	B	550	TYR	3.1
1	A	926	GLY	3.1
1	B	928	ASN	3.0
1	A	949	ALA	3.0
1	A	594[A]	ARG	3.0
1	B	925	ASN	3.0
1	A	840	GLU	3.0
1	B	551	VAL	2.9
1	A	900	ASN	2.8
1	A	550	TYR	2.8
1	A	546	ASP	2.7
1	B	532	ILE	2.7
1	B	545	GLN	2.7
1	B	659	THR	2.7
1	B	601	ALA	2.7
1	A	838	SER	2.5
1	A	544	LYS	2.5
1	B	722	ASN	2.5
1	A	659	THR	2.5
1	B	839	PRO	2.5
1	B	595	SER	2.4
1	A	925	ASN	2.4
1	B	524	ALA	2.4
1	B	547	ASP	2.4
1	A	605	THR	2.4
1	A	896	VAL	2.4
1	A	901	PHE	2.3
1	A	906	ILE	2.3
1	B	711	GLU	2.3
1	B	531	ILE	2.2
1	B	949	ALA	2.2
1	B	546	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	842	ALA	2.1
1	B	838	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

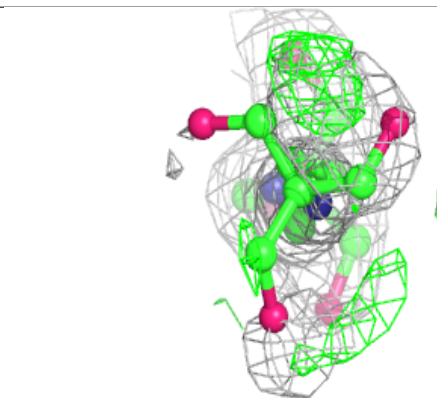
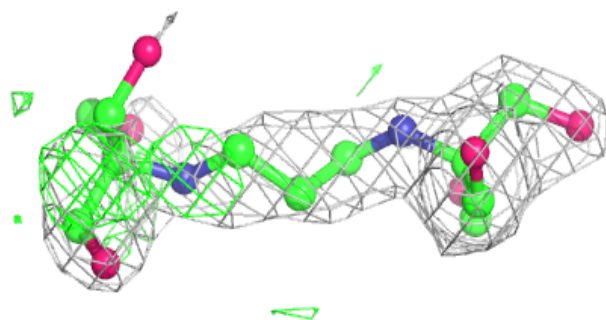
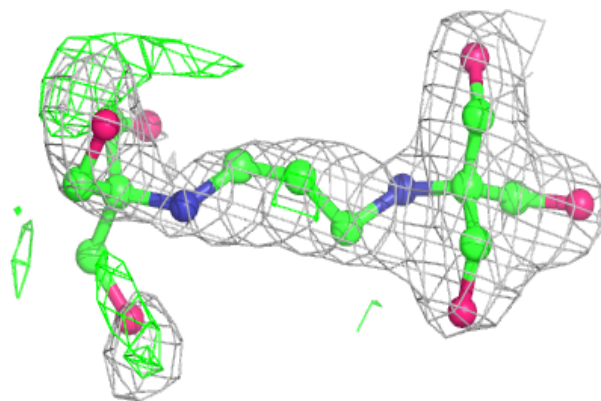
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	B3P	A	1003	19/19	0.82	0.19	50,62,68,69	8
4	B3P	B	1003	19/19	0.88	0.16	51,64,68,72	9
2	CEP	B	1001	22/26	0.93	0.11	39,50,65,71	0
3	SCN	B	1002	3/3	0.94	0.19	33,33,58,65	0
3	SCN	A	1002	3/3	0.96	0.10	38,38,51,56	0
2	CEP	A	1001[B]	22/26	0.96	0.12	34,45,73,82	5
2	CEP	A	1001[A]	22/26	0.96	0.12	34,45,92,97	5

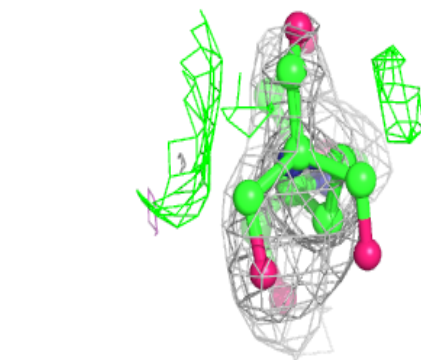
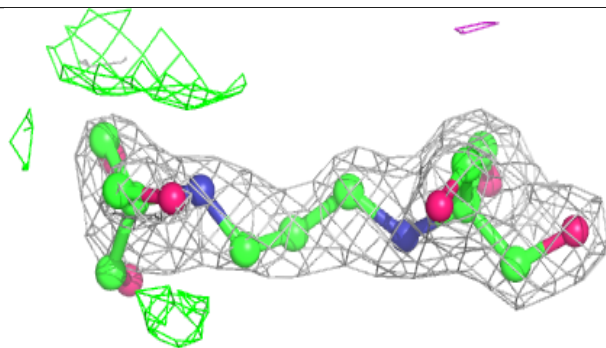
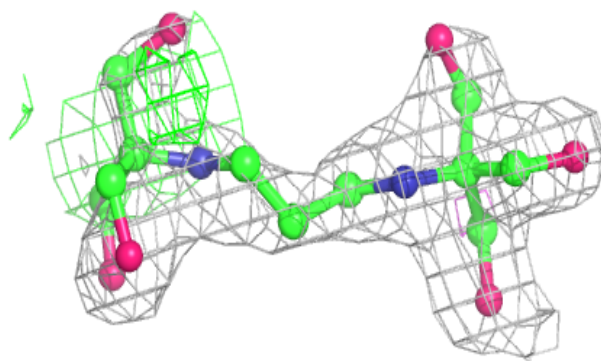
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around B3P A 1003:**

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

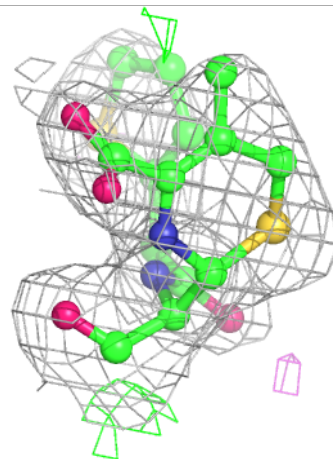
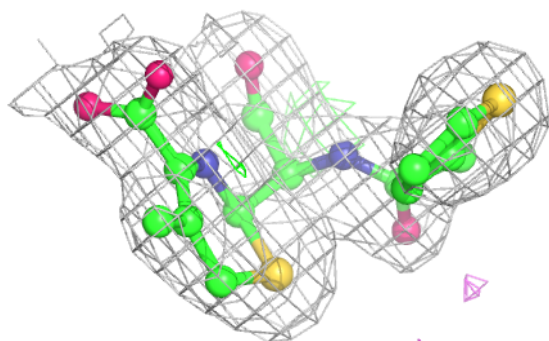
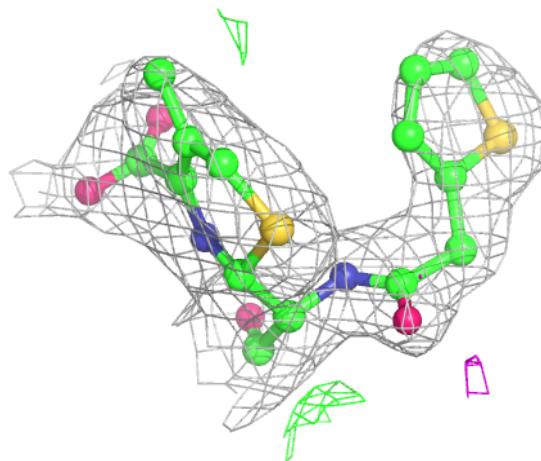
**Electron density around B3P B 1003:**

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



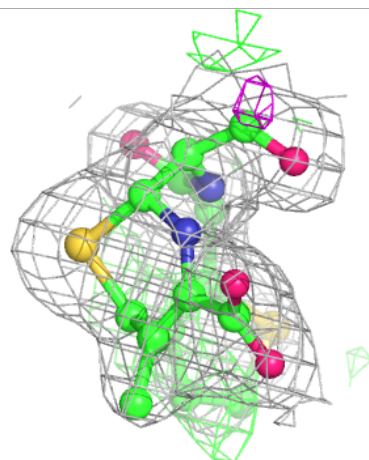
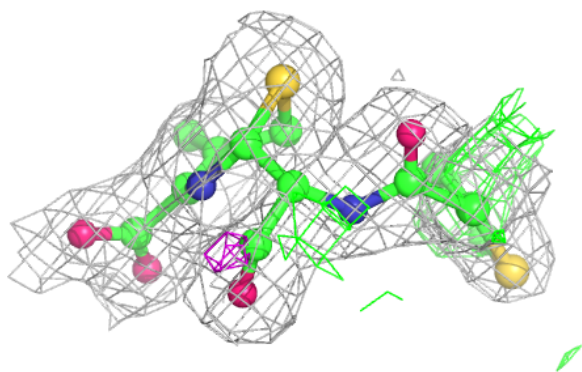
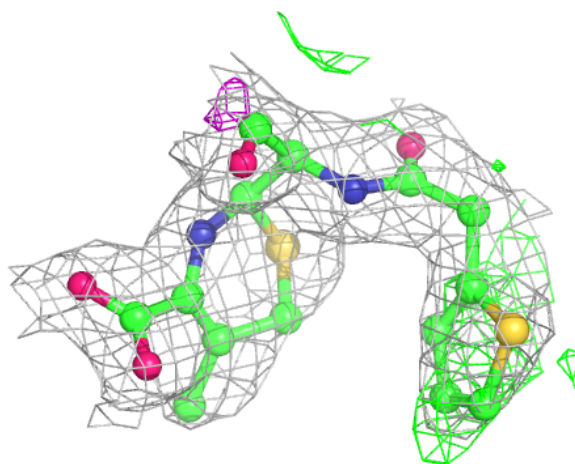
**Electron density around CEP B 1001:**

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



**Electron density around CEP A 1001 (B):**

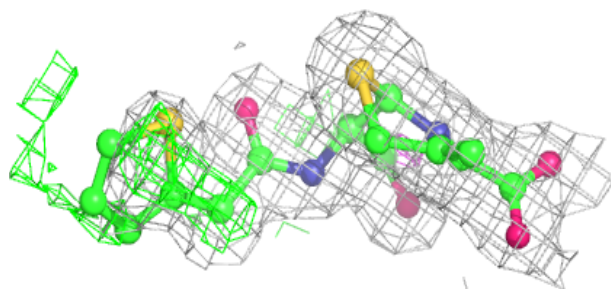
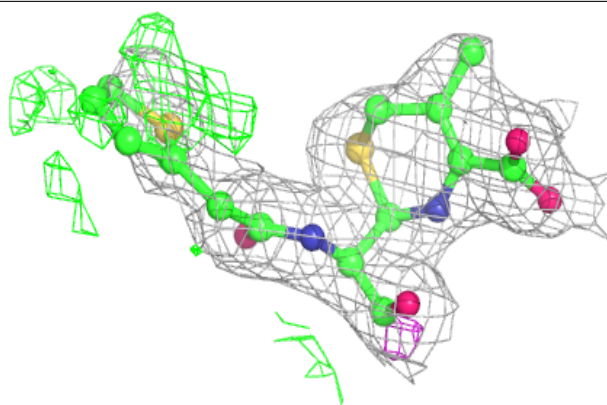
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CEP A 1001 (A):**

$2mF_o - DF_c$  (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.