



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:28 pm BST

PDB ID : 2Y2G  
Title : PENICILLIN-BINDING PROTEIN 1B (PBP-1B) IN COMPLEX WITH AN ALKYL BORONATE (A01)  
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Deposited on : 2010-12-15  
Resolution : 2.05 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

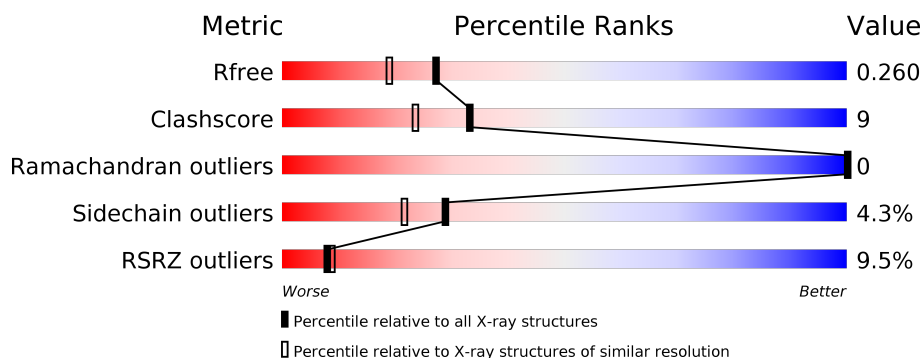
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	494	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	494	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>

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
4	CL	A	1204	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7930 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.

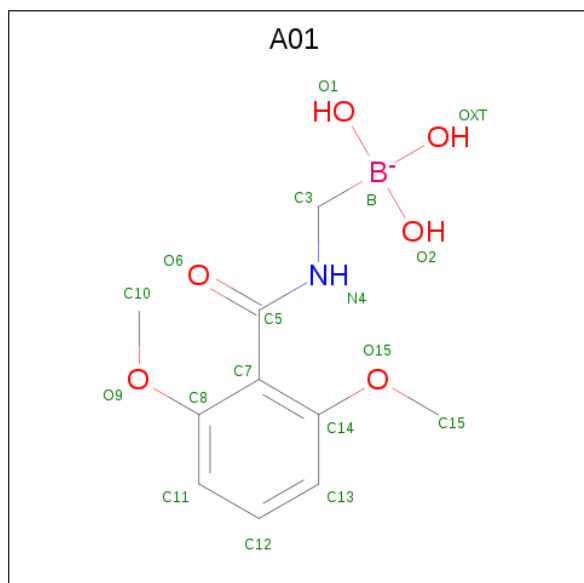
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	2	0
			3610	2260	614	721	15			
1	B	466	Total	C	N	O	S	0	1	0
			3603	2255	613	720	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	ASN	engineered mutation	UNP Q7CRA4
A	686	GLN	ARG	engineered mutation	UNP Q7CRA4
A	687	GLN	ARG	engineered mutation	UNP Q7CRA4
B	656	GLY	ASN	engineered mutation	UNP Q7CRA4
B	686	GLN	ARG	engineered mutation	UNP Q7CRA4
B	687	GLN	ARG	engineered mutation	UNP Q7CRA4

- Molecule 2 is [(2,6-DIMETHOXYPHENYL)CARBONYLAMINO]METHYL-TRIHYDROXY-BORON (three-letter code: A01) (formula: C<sub>10</sub>H<sub>15</sub>BNO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			17	1	10	1	5		
2	B	1	Total	B	C	N	O	0	0
			17	1	10	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	17	Total	Cl	0	0
			17	17		
4	A	13	Total	Cl	0	0
			13	13		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

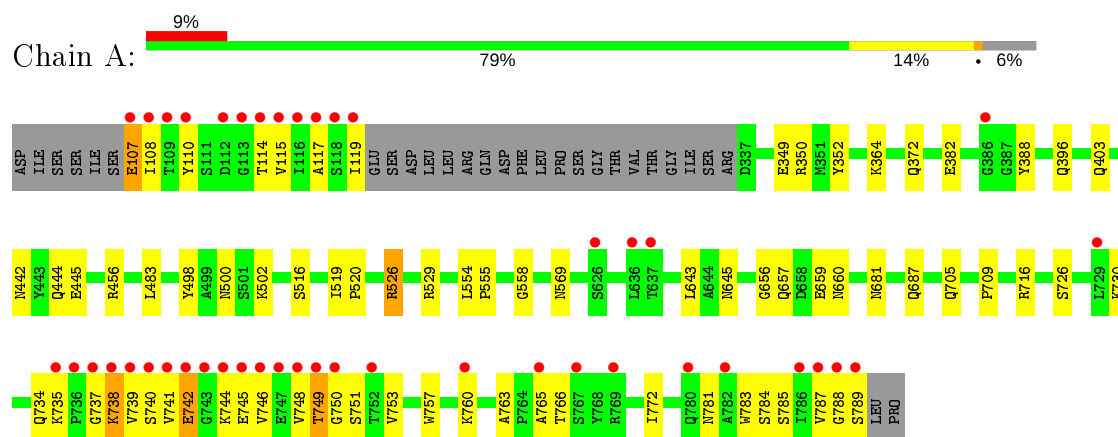
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	318	Total	O	0	0
			318	318		
7	B	307	Total	O	0	0
			307	307		

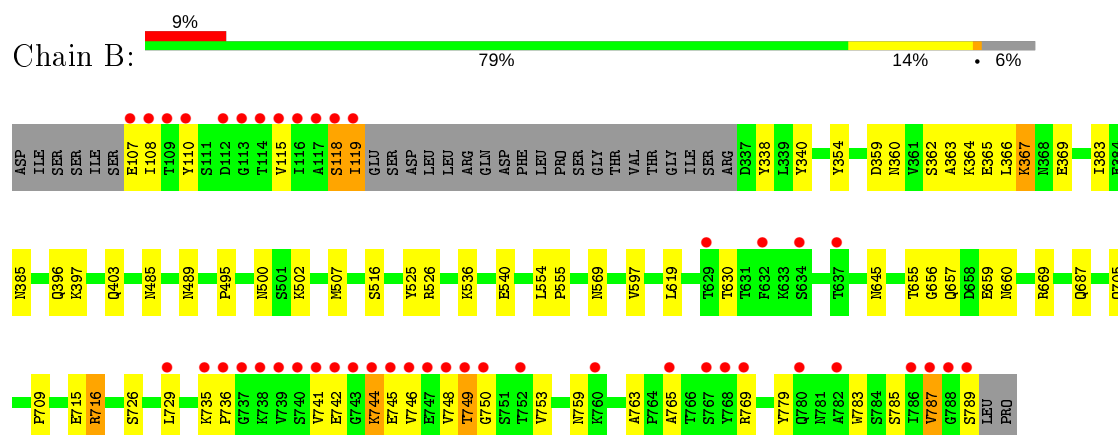
### 3 Residue-property plots [i](#)

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: PENICILLIN-BINDING PROTEIN 1B



#### • Molecule 1: PENICILLIN-BINDING PROTEIN 1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.53Å 97.53Å 149.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.05 48.76 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.3 (48.74-2.05) 90.4 (48.76-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, $R_{free}$	0.222 , 0.260 0.223 , 0.260	Depositor DCC
$R_{free}$ test set	4088 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6408e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, A01, EDO, CL

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	0/3686	0.51	0/5001
1	B	0.47	0/3676	0.51	0/4989
All	All	0.47	0/7362	0.51	0/9990

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3610	0	3486	57	0
1	B	3603	0	3470	64	0
2	A	17	0	13	3	0
2	B	17	0	13	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	13	0	0	2	0
4	B	17	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	12	3	0
7	A	318	0	0	6	0
7	B	307	0	0	16	0
All	All	7930	0	7006	123	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 9.

All (123) 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:442:ASN:ND2	1:A:445:GLU:HG2	1.69	1.05
1:A:526[B]:ARG:HD3	7:A:2176:HOH:O	1.65	0.97
1:B:729:LEU:HD11	1:B:736:PRO:HA	1.47	0.96
1:B:687:GLN:HB2	7:B:2242:HOH:O	1.68	0.92
1:B:741:VAL:O	1:B:742:GLU:HG2	1.73	0.88
1:A:645:ASN:O	1:A:716:ARG:NH2	2.09	0.85
1:B:107:GLU:HG3	1:B:115:VAL:HG13	1.61	0.82
1:A:730[A]:LYS:HG3	1:A:753:VAL:HG13	1.62	0.78
1:B:107:GLU:HG3	1:B:115:VAL:CG1	2.13	0.77
1:A:502:LYS:HE2	7:A:2126:HOH:O	1.85	0.77
1:A:442:ASN:ND2	1:A:445:GLU:CG	2.47	0.76
1:B:107:GLU:HA	7:B:2001:HOH:O	1.86	0.75
1:B:742:GLU:O	1:B:742:GLU:HG3	1.87	0.74
1:B:500:ASN:HB2	7:B:2111:HOH:O	1.86	0.74
1:B:110:TYR:CG	1:B:396:GLN:HB2	2.23	0.73
1:A:687:GLN:HB2	7:A:2255:HOH:O	1.88	0.73
1:B:365:GLU:HB3	7:B:2020:HOH:O	1.89	0.72
1:B:525:TYR:CD2	1:B:526[B]:ARG:NH1	2.59	0.69
1:B:107:GLU:CG	1:B:115:VAL:HG13	2.24	0.68
1:B:645:ASN:O	1:B:716:ARG:NH2	2.26	0.67
1:B:119:ILE:HG23	1:B:340:TYR:OH	1.94	0.66
1:B:741:VAL:O	1:B:742:GLU:CG	2.44	0.64
1:B:397:LYS:HE3	7:B:2033:HOH:O	1.98	0.63
1:B:110:TYR:CD2	1:B:396:GLN:HB2	2.34	0.62
1:A:526[B]:ARG:NH1	1:A:529:ARG:HG3	2.14	0.61
1:B:526[B]:ARG:HD3	7:B:2139:HOH:O	1.99	0.61
1:A:554:LEU:N	1:A:555:PRO:HD2	2.16	0.61
1:B:489:ASN:HD22	1:B:495:PRO:HA	1.67	0.60
1:B:749:THR:HG23	1:B:750:GLY:N	2.17	0.60
1:B:716:ARG:HD3	7:B:2271:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:HG2	7:B:2023:HOH:O	2.02	0.59
1:B:362:SER:OG	1:B:365:GLU:HG3	2.01	0.59
1:B:729:LEU:CD1	1:B:736:PRO:HA	2.25	0.59
2:B:1000:A01:H12	7:B:2244:HOH:O	2.01	0.58
1:A:749:THR:HG23	1:A:750:GLY:N	2.18	0.58
1:A:352:TYR:OH	1:A:372:GLN:HG2	2.03	0.58
1:A:526[B]:ARG:HH11	1:A:529:ARG:HG3	1.69	0.57
1:A:735:LYS:HB2	1:A:765:ALA:HA	1.87	0.57
1:B:502:LYS:HE2	7:B:2117:HOH:O	2.05	0.56
1:B:526[B]:ARG:CD	7:B:2139:HOH:O	2.53	0.56
1:B:779:TYR:O	1:B:783:TRP:HD1	1.89	0.56
1:B:110:TYR:CD1	1:B:396:GLN:HB2	2.41	0.56
1:A:783:TRP:O	1:A:787:VAL:HB	2.06	0.55
1:B:359:ASP:O	1:B:360:ASN:HB2	2.06	0.55
1:A:656:GLY:O	2:A:1000:A01:H151	2.07	0.55
1:A:738:LYS:HA	1:A:746:VAL:O	2.08	0.54
1:A:705:GLN:HE22	6:A:1401:EDO:H22	1.73	0.54
1:B:363:ALA:O	1:B:367:LYS:HD2	2.07	0.54
1:A:657:GLN:HB2	1:A:659:GLU:CD	2.28	0.53
1:B:554:LEU:N	1:B:555:PRO:HD2	2.23	0.53
1:B:107:GLU:CA	7:B:2001:HOH:O	2.50	0.53
1:B:118:SER:C	1:B:119:ILE:HG12	2.28	0.53
1:A:785:SER:O	1:A:788:GLY:N	2.41	0.53
1:A:705:GLN:OE1	6:A:1401:EDO:H11	2.09	0.53
1:A:781:ASN:O	1:A:784:SER:HB3	2.09	0.52
1:A:110:TYR:CG	1:A:396:GLN:HB2	2.45	0.52
1:B:354:TYR:CG	1:B:597:VAL:HG13	2.46	0.51
1:A:442:ASN:HD21	1:A:445:GLU:HG2	1.71	0.51
1:B:729:LEU:HD21	1:B:736:PRO:HB3	1.93	0.51
1:B:735:LYS:HD2	1:B:763:ALA:O	2.10	0.51
1:B:657:GLN:HB2	1:B:659:GLU:CD	2.32	0.51
1:B:769:ARG:HA	1:B:779:TYR:CE1	2.46	0.50
1:A:730[A]:LYS:HD2	1:A:751:SER:OG	2.11	0.50
1:B:655:THR:HG21	1:B:660:ASN:HD22	1.76	0.50
1:A:456:ARG:HD2	1:A:660:ASN:OD1	2.12	0.49
1:B:759:ASN:HB2	4:B:1203:CL:CL	2.49	0.49
1:A:108:ILE:HD12	1:A:119:ILE:HD11	1.92	0.49
1:A:403:GLN:NE2	7:A:2037:HOH:O	2.42	0.49
1:B:619:LEU:HD23	6:B:1400:EDO:H11	1.94	0.49
1:B:705:GLN:HE22	6:B:1401:EDO:H22	1.77	0.48
1:A:108:ILE:CD1	1:A:119:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:CG2	1:B:340:TYR:OH	2.62	0.48
1:A:554:LEU:N	1:A:555:PRO:CD	2.75	0.48
1:B:656:GLY:O	2:B:1000:A01:H151	2.13	0.48
1:A:442:ASN:HD22	1:A:445:GLU:CG	2.25	0.48
1:A:498:TYR:OH	2:A:1000:A01:H103	2.14	0.47
1:A:107:GLU:HG3	1:A:115:VAL:HG13	1.96	0.47
1:A:110:TYR:CD2	1:A:396:GLN:HB2	2.49	0.47
1:A:741:VAL:C	1:A:742:GLU:HG3	2.35	0.47
1:B:525:TYR:CE2	1:B:526[B]:ARG:NH1	2.82	0.46
1:A:110:TYR:HB3	4:A:1216:CL:CL	2.53	0.46
1:B:525:TYR:HD2	1:B:526[B]:ARG:HH11	1.63	0.46
1:B:687:GLN:HG2	7:B:2246:HOH:O	2.16	0.46
1:B:741:VAL:C	1:B:742:GLU:HG2	2.36	0.46
1:B:525:TYR:HD2	1:B:526[B]:ARG:NH1	2.09	0.45
1:A:382:GLU:HG3	1:A:388:TYR:CE1	2.50	0.45
1:A:107:GLU:HB2	1:A:117:ALA:O	2.17	0.45
1:A:498:TYR:CZ	2:A:1000:A01:H103	2.52	0.45
1:A:350:ARG:HA	1:A:350:ARG:HD3	1.78	0.44
1:A:738:LYS:HD2	1:A:745:GLU:OE2	2.17	0.44
1:B:779:TYR:O	1:B:783:TRP:CD1	2.70	0.44
1:A:739:VAL:CG1	1:A:740:SER:N	2.80	0.44
1:A:114:THR:HG21	1:A:396:GLN:OE1	2.18	0.44
1:A:519:ILE:N	1:A:520:PRO:CD	2.81	0.44
1:B:338:TYR:HB2	4:B:1213:CL:CL	2.55	0.44
1:B:403:GLN:NE2	7:B:2038:HOH:O	2.34	0.44
1:A:737:GLY:O	1:A:748:VAL:HG23	2.17	0.43
1:B:705:GLN:O	1:B:709:PRO:HA	2.18	0.43
1:B:783:TRP:O	1:B:787:VAL:HB	2.17	0.43
1:B:669:ARG:NH2	1:B:715:GLU:OE2	2.51	0.43
1:A:643:LEU:HD13	1:A:705:GLN:HG3	2.00	0.43
1:B:108:ILE:HD11	1:B:119:ILE:CD1	2.49	0.43
1:A:483:LEU:HD23	1:A:772:ILE:HB	2.01	0.42
1:B:536:LYS:O	1:B:540:GLU:HG3	2.18	0.42
1:A:500:ASN:HB2	7:A:2121:HOH:O	2.19	0.42
1:B:107:GLU:HG3	1:B:115:VAL:HG11	1.96	0.42
1:A:760:LYS:HB2	4:A:1203:CL:CL	2.57	0.42
1:B:729:LEU:HD13	1:B:748:VAL:HG12	2.01	0.42
2:B:1000:A01:C12	7:B:2244:HOH:O	2.66	0.42
1:A:757:TRP:NE1	1:A:763:ALA:HB2	2.35	0.41
1:A:734:GLN:OE1	1:A:766:THR:HA	2.19	0.41
1:B:735:LYS:HB2	1:B:765:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLN:O	1:A:709:PRO:HA	2.20	0.41
1:B:705:GLN:OE1	6:B:1401:EDO:H11	2.21	0.41
1:A:110:TYR:CD1	1:A:396:GLN:HB2	2.56	0.41
1:A:526[A]:ARG:NE	7:A:2149:HOH:O	2.53	0.41
1:A:657:GLN:HB2	1:A:659:GLU:OE2	2.20	0.41
1:B:744:LYS:O	1:B:746:VAL:HG23	2.21	0.41
1:A:787:VAL:O	1:A:787:VAL:CG1	2.69	0.41
1:A:741:VAL:O	1:A:742:GLU:HG3	2.21	0.40
1:B:118:SER:HA	7:B:2001:HOH:O	2.21	0.40
1:A:554:LEU:HD12	1:A:558:GLY:O	2.22	0.40
1:B:485:ASN:HB3	1:B:507:MET:HE3	2.04	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	464/494 (94%)	450 (97%)	14 (3%)	0	100	100
1	B	463/494 (94%)	442 (96%)	21 (4%)	0	100	100
All	All	927/988 (94%)	892 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/408 (94%)	369 (96%)	15 (4%)	32	25
1	B	382/408 (94%)	363 (95%)	19 (5%)	24	16
All	All	766/816 (94%)	732 (96%)	34 (4%)	29	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	349	GLU
1	A	364	LYS
1	A	444	GLN
1	A	516	SER
1	A	526[A]	ARG
1	A	526[B]	ARG
1	A	569	ASN
1	A	681	ASN
1	A	726	SER
1	A	738	LYS
1	A	742	GLU
1	A	744	LYS
1	A	749	THR
1	A	789	SER
1	B	118	SER
1	B	119	ILE
1	B	364	LYS
1	B	366	LEU
1	B	367	LYS
1	B	383	ILE
1	B	385	ASN
1	B	516	SER
1	B	569	ASN
1	B	630	THR
1	B	716	ARG
1	B	726	SER
1	B	744	LYS
1	B	745	GLU
1	B	749	THR
1	B	753	VAL
1	B	785	SER
1	B	787	VAL
1	B	789	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	A	692	ASN
1	B	448	ASN
1	B	489	ASN
1	B	657	GLN
1	B	692	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 ⓘ

Of 40 ligands modelled in this entry, 32 are monoatomic - leaving 8 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	$\# Z  > 2$
6	EDO	B	1401	-	3,3,3	0.52	0	2,2,2	0.44	0
6	EDO	A	1401	-	3,3,3	0.49	0	2,2,2	0.41	0
6	EDO	B	1400	-	3,3,3	0.43	0	2,2,2	0.47	0
2	A01	A	1000	1,5	15,17,18	1.94	2 (13%)	18,22,25	1.82	5 (27%)
3	SO4	B	1100	-	4,4,4	0.51	0	6,6,6	0.39	0
3	SO4	A	1100	-	4,4,4	0.46	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	1400	-	3,3,3	0.48	0	2,2,2	0.44	0
2	A01	B	1000	1,5	15,17,18	1.93	1 (6%)	18,22,25	1.75	4 (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
6	EDO	B	1401	-	-	0/1/1/1	-
6	EDO	A	1401	-	-	1/1/1/1	-
6	EDO	B	1400	-	-	1/1/1/1	-
2	A01	A	1000	1,5	-	6/10/13/14	0/1/1/1
6	EDO	A	1400	-	-	0/1/1/1	-
2	A01	B	1000	1,5	-	4/10/13/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	A01	C3-N4	-7.05	1.36	1.46
2	A	1000	A01	C3-N4	-6.91	1.36	1.46
2	A	1000	A01	C7-C5	2.19	1.54	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	A01	O15-C14-C7	4.05	121.50	115.85
2	B	1000	A01	O15-C14-C7	3.99	121.40	115.85
2	A	1000	A01	O15-C14-C13	-3.72	117.99	124.37
2	B	1000	A01	O15-C14-C13	-3.28	118.74	124.37
2	B	1000	A01	C10-O9-C8	3.27	122.46	117.53
2	A	1000	A01	C10-O9-C8	3.07	122.17	117.53
2	A	1000	A01	O9-C8-C7	3.01	120.05	115.85
2	A	1000	A01	O9-C8-C11	-2.60	119.92	124.37
2	B	1000	A01	O9-C8-C7	2.50	119.34	115.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	A01	O6-C5-C7-C14

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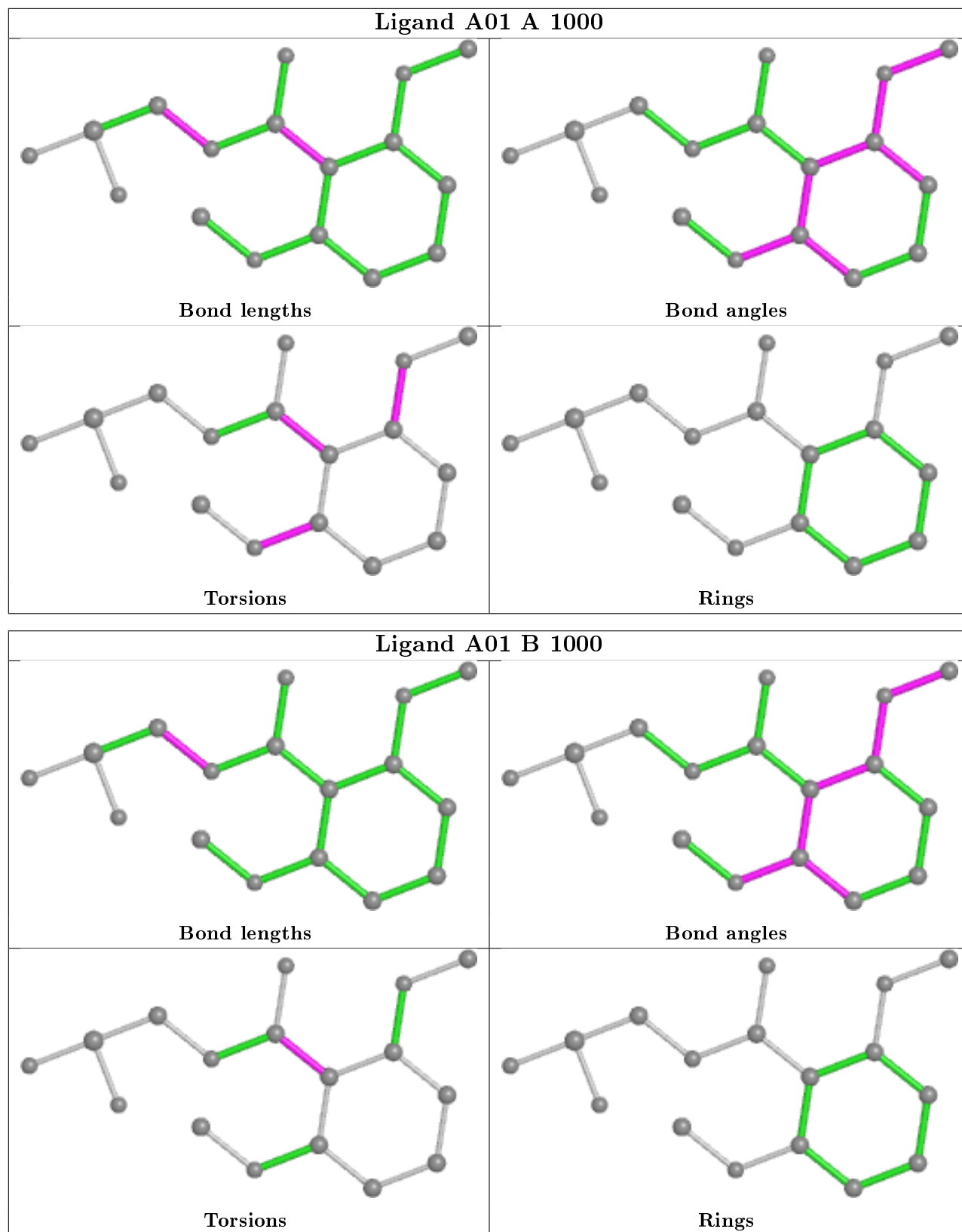
Mol	Chain	Res	Type	Atoms
2	A	1000	A01	O6-C5-C7-C8
2	B	1000	A01	N4-C5-C7-C8
2	B	1000	A01	N4-C5-C7-C14
2	A	1000	A01	N4-C5-C7-C8
2	A	1000	A01	C7-C14-O15-C15
6	B	1400	EDO	O1-C1-C2-O2
6	A	1401	EDO	O1-C1-C2-O2
2	A	1000	A01	C11-C8-O9-C10
2	B	1000	A01	O6-C5-C7-C8
2	A	1000	A01	C13-C14-O15-C15
2	A	1000	A01	C7-C8-O9-C10

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1401	EDO	2	0
6	A	1401	EDO	2	0
6	B	1400	EDO	1	0
2	A	1000	A01	3	0
2	B	1000	A01	3	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 ⓘ

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, 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	466/494 (94%)	0.40	44 (9%) <b>8</b> <b>9</b>	25, 42, 85, 134	0
1	B	466/494 (94%)	0.43	45 (9%) <b>7</b> <b>8</b>	24, 42, 86, 145	0
All	All	932/988 (94%)	0.42	89 (9%) <b>8</b> <b>9</b>	24, 42, 86, 145	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	744	LYS	7.2
1	B	787	VAL	6.9
1	A	738	LYS	6.9
1	B	117	ALA	6.1
1	B	744	LYS	5.9
1	A	787	VAL	5.7
1	A	117	ALA	5.5
1	B	738	LYS	5.4
1	A	115	VAL	5.4
1	B	746	VAL	5.1
1	B	739	VAL	5.0
1	B	119	ILE	4.8
1	A	739	VAL	4.8
1	A	737	GLY	4.7
1	B	115	VAL	4.7
1	A	119	ILE	4.6
1	B	118	SER	4.6
1	A	746	VAL	4.5
1	B	114	THR	4.5
1	B	737	GLY	4.5
1	B	743	GLY	4.4
1	B	748	VAL	4.3
1	A	740	SER	4.1
1	B	116	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	743	GLY	4.0
1	B	736	PRO	3.9
1	A	742	GLU	3.8
1	B	750	GLY	3.8
1	A	780	GLN	3.8
1	A	736	PRO	3.7
1	B	780	GLN	3.7
1	B	110	TYR	3.5
1	A	748	VAL	3.5
1	B	113	GLY	3.5
1	A	786	ILE	3.5
1	A	745	GLU	3.4
1	B	786	ILE	3.2
1	B	742	GLU	3.2
1	A	735	LYS	3.2
1	A	741	VAL	3.2
1	A	113	GLY	3.1
1	A	116	ILE	3.1
1	B	741	VAL	3.1
1	B	789	SER	3.1
1	A	788	GLY	3.0
1	B	108	ILE	3.0
1	B	109	THR	3.0
1	A	118	SER	3.0
1	A	749	THR	2.9
1	B	107	GLU	2.9
1	B	745	GLU	2.9
1	B	747	GLU	2.9
1	A	112	ASP	2.8
1	A	109	THR	2.8
1	A	108	ILE	2.8
1	A	107	GLU	2.6
1	A	760	LYS	2.6
1	A	110	TYR	2.6
1	A	747	GLU	2.6
1	B	749	THR	2.6
1	B	735	LYS	2.6
1	B	740	SER	2.6
1	A	114	THR	2.5
1	A	750	GLY	2.5
1	B	752	THR	2.5
1	A	767	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	782	ALA	2.4
1	B	729	LEU	2.4
1	A	752	THR	2.4
1	B	765	ALA	2.3
1	B	767	SER	2.3
1	B	760	LYS	2.2
1	B	112	ASP	2.2
1	B	788	GLY	2.2
1	B	769	ARG	2.2
1	A	765	ALA	2.2
1	B	637	THR	2.2
1	B	632	PHE	2.2
1	B	768	TYR	2.2
1	A	626	SER	2.2
1	A	769	ARG	2.1
1	A	386	GLY	2.1
1	A	637	THR	2.1
1	B	782	ALA	2.1
1	A	729	LEU	2.1
1	B	629	THR	2.1
1	A	789	SER	2.0
1	A	636	LEU	2.0
1	B	634	SER	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. 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.

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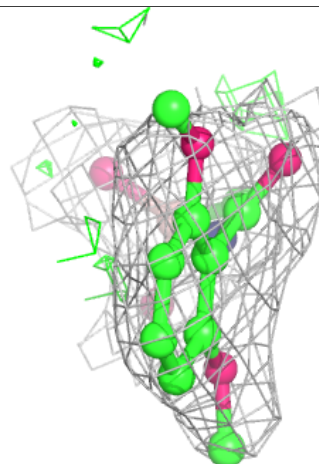
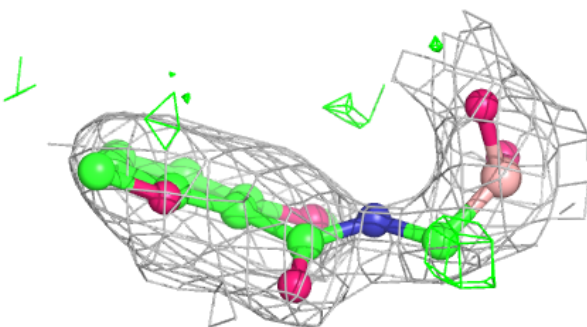
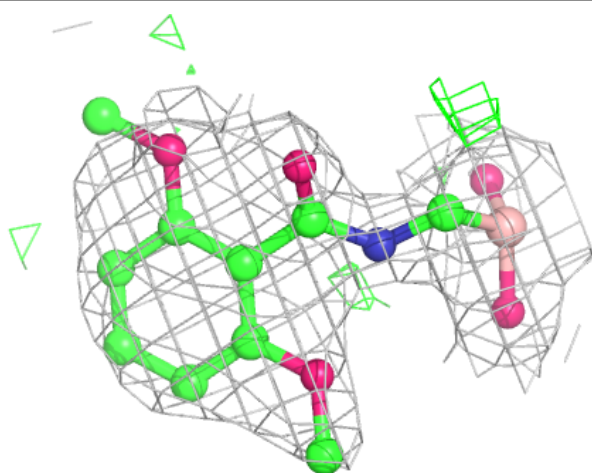
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	1208	1/1	0.78	0.23	71,71,71,71	0
4	CL	A	1204	1/1	0.79	0.42	77,77,77,77	0
4	CL	B	1206	1/1	0.79	0.31	78,78,78,78	0
4	CL	A	1216	1/1	0.83	0.19	67,67,67,67	0
4	CL	A	1203	1/1	0.86	0.23	75,75,75,75	0
6	EDO	A	1401	4/4	0.87	0.12	53,57,59,70	0
4	CL	B	1216	1/1	0.88	0.17	69,69,69,69	0
6	EDO	B	1401	4/4	0.88	0.14	39,55,59,61	0
4	CL	A	1208	1/1	0.89	0.30	73,73,73,73	0
4	CL	B	1203	1/1	0.90	0.29	76,76,76,76	0
4	CL	A	1214	1/1	0.92	0.10	64,64,64,64	0
4	CL	A	1202	1/1	0.92	0.25	64,64,64,64	0
4	CL	B	1792	1/1	0.93	0.27	40,40,40,40	1
4	CL	A	1206	1/1	0.93	0.13	56,56,56,56	0
4	CL	B	1234	1/1	0.93	0.11	56,56,56,56	0
2	A01	B	1000	17/18	0.94	0.16	43,65,90,101	0
2	A01	A	1000	17/18	0.94	0.13	35,59,84,105	0
4	CL	B	1235	1/1	0.94	0.28	60,60,60,60	0
6	EDO	A	1400	4/4	0.95	0.12	42,45,49,52	0
4	CL	B	1202	1/1	0.95	0.19	62,62,62,62	0
6	EDO	B	1400	4/4	0.96	0.14	38,49,54,60	0
4	CL	B	1214	1/1	0.96	0.12	57,57,57,57	0
4	CL	A	1201	1/1	0.96	0.09	47,47,47,47	0
4	CL	B	1200	1/1	0.96	0.10	47,47,47,47	0
4	CL	A	1200	1/1	0.97	0.08	51,51,51,51	0
5	NA	B	1300	1/1	0.97	0.21	37,37,37,37	0
5	NA	A	1300	1/1	0.97	0.26	40,40,40,40	0
4	CL	B	1201	1/1	0.98	0.09	48,48,48,48	0
4	CL	A	1213	1/1	0.98	0.09	60,60,60,60	0
3	SO4	B	1100	5/5	0.98	0.07	42,44,52,54	0
4	CL	A	1212	1/1	0.98	0.07	48,48,48,48	0
4	CL	A	1229	1/1	0.99	0.06	59,59,59,59	0
3	SO4	A	1100	5/5	0.99	0.08	38,41,45,57	0
4	CL	B	1213	1/1	0.99	0.12	53,53,53,53	0
4	CL	B	1224	1/1	0.99	0.11	59,59,59,59	0
4	CL	B	1229	1/1	0.99	0.08	55,55,55,55	0
4	CL	B	1212	1/1	0.99	0.08	43,43,43,43	0
4	CL	A	1211	1/1	0.99	0.09	40,40,40,40	0
4	CL	B	1211	1/1	1.00	0.10	44,44,44,44	0
4	CL	B	1791	1/1	1.00	0.21	29,29,29,29	0

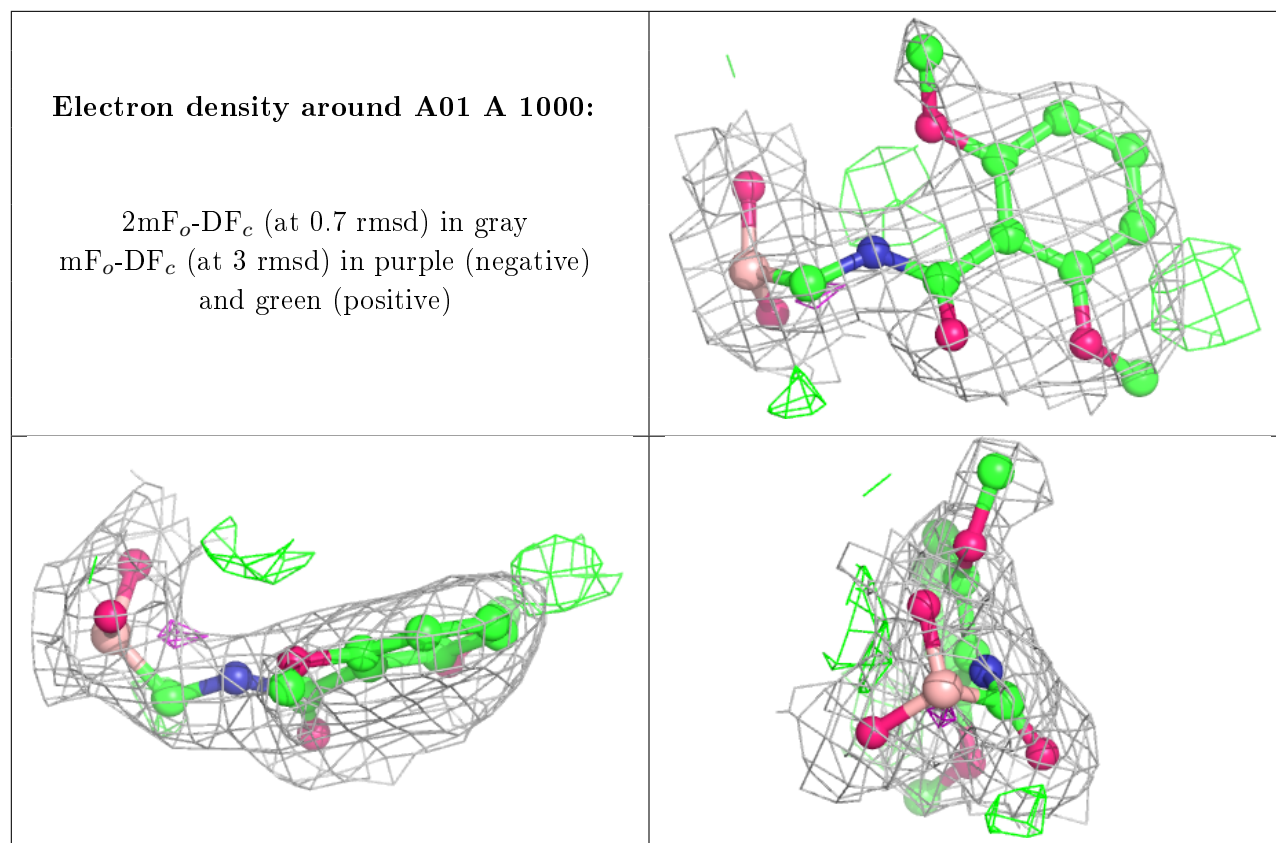
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A01 B 1000:**

$2mF_o-DF_c$  (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.