



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 08:04 PM JST

PDB ID : 4YCM / pdb\_00004ycm  
Title : Crystal structure of the calcium pump with bound marine macrolide BLS  
Authors : Morita, M.; Ogawa, H.; Ohno, O.; Yamori, T.; Suenaga, K.; Toyoshima, C.  
Deposited on : 2015-02-20  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

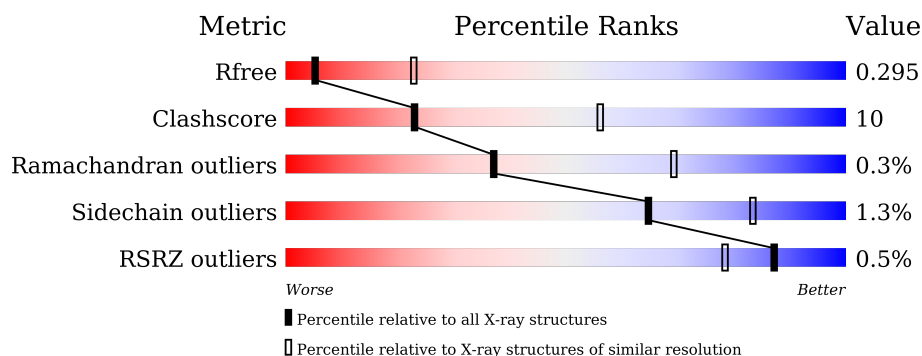
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	994	<div> <div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="margin-left: 10px;"> <div style="width: 100%; height: 10px; background-color: red;"></div> </div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>78%</span> <span>22%</span> <span>.</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7818 atoms, of which 52 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.

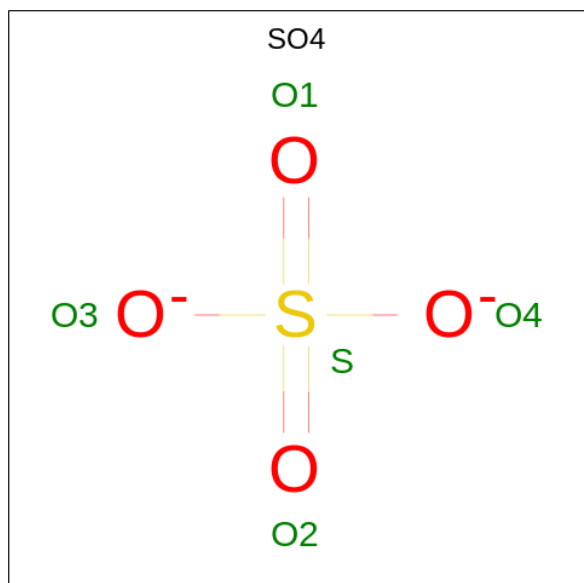
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

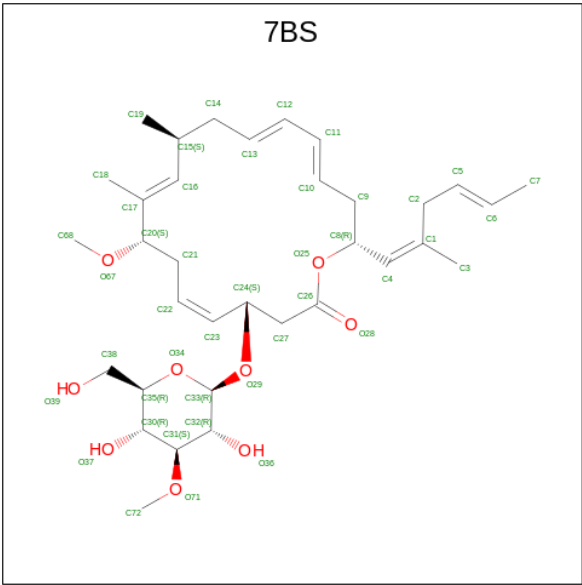
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



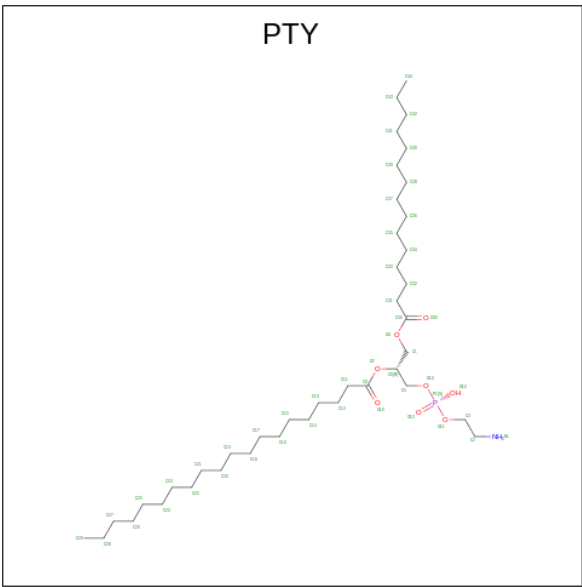
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (4S,5E,8S,9E,11S,13E,15E,18R)-8-methoxy-9,11-dimethyl-18-[(1Z,4E)-2-methylhexa-1,4-dien-1-yl]-2-oxooxacyclooctadeca-5,9,13,15-tetraen-4-yl 3-O-methyl-beta-D-glucopyranoside (CCD ID: 7BS) (formula: C<sub>34</sub>H<sub>52</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	95	34	52	9	0	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0

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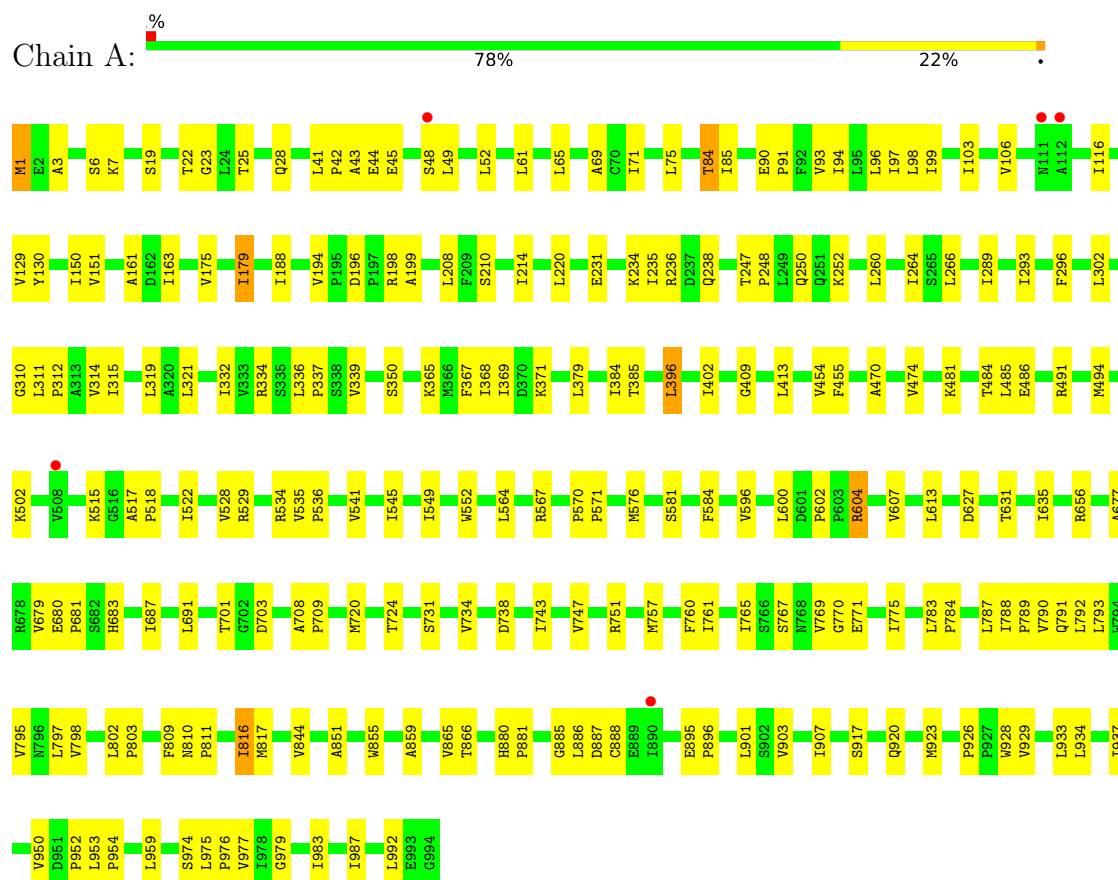
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

### 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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.67Å 71.67Å 585.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.97 – 3.20 15.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (15.97-3.20) 98.6 (15.97-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.215 , 0.260 0.242 , 0.295	Depositor DCC
$R_{free}$ test set	841 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: AME, PTY, 7BS, NA, SO4

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	0.20	0/7804	0.36	0/10582

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 [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	7674	0	7765	159	0
2	A	1	0	0	0	0
3	A	10	0	0	0	0
4	A	43	52	52	3	0
5	A	38	0	22	1	0
All	All	7766	52	7839	159	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 10.

All (159) 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:950:VAL:HG12	1:A:952:PRO:HD2	1.56	0.85
1:A:757:MET:HA	1:A:760:PHE:CE2	2.17	0.78
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.68	0.75
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.73	0.71
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.73	0.69
1:A:84:THR:HG23	1:A:85:ILE:H	1.58	0.69
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.75	0.67
1:A:48:SER:HB2	1:A:52:LEU:HD22	1.77	0.67
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.77	0.66
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.78	0.65
1:A:337:PRO:HG3	4:A:1004:7BS:H47	1.79	0.65
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.80	0.64
1:A:179:ILE:HD13	1:A:179:ILE:H	1.61	0.64
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.27	0.63
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.81	0.61
1:A:175:VAL:HG11	1:A:208:LEU:HD22	1.81	0.61
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.83	0.60
1:A:248:PRO:O	1:A:252:LYS:HG2	2.01	0.60
1:A:816:ILE:O	1:A:816:ILE:HD13	2.02	0.59
1:A:319:LEU:HD11	1:A:757:MET:CE	2.34	0.58
1:A:844:VAL:HG12	1:A:907:ILE:HG21	1.87	0.57
1:A:486:GLU:O	1:A:491:ARG:NH2	2.38	0.57
1:A:600:LEU:O	1:A:602:PRO:HD3	2.04	0.56
1:A:880:HIS:N	1:A:881:PRO:HD2	2.20	0.56
1:A:97:ILE:HD11	1:A:797:LEU:HD21	1.87	0.56
1:A:336:LEU:O	1:A:339:VAL:HG22	2.05	0.56
1:A:788:ILE:HG22	1:A:790:VAL:H	1.70	0.56
1:A:65:LEU:CD2	1:A:94:ILE:HG23	2.36	0.56
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.88	0.55
1:A:196:ASP:HB3	1:A:199:ALA:HB2	1.88	0.55
1:A:703:ASP:O	1:A:724:THR:HG22	2.07	0.55
1:A:48:SER:CB	1:A:52:LEU:HD22	2.36	0.55
1:A:103:ILE:HA	1:A:106:VAL:HG12	1.89	0.54
1:A:604:ARG:CB	1:A:607:VAL:HG13	2.38	0.54
1:A:6:SER:HA	1:A:194:VAL:O	2.08	0.54
1:A:751:ARG:HD2	1:A:817:MET:CE	2.38	0.53
1:A:234:LYS:O	1:A:238:GLN:HG3	2.09	0.53
1:A:99:ILE:O	1:A:103:ILE:HG13	2.08	0.53
1:A:247:THR:HG23	1:A:250:GLN:HG3	1.91	0.53
1:A:188:ILE:HD12	1:A:188:ILE:N	2.25	0.52
1:A:151:VAL:CG2	1:A:163:ILE:HD13	2.38	0.52
1:A:751:ARG:HD2	1:A:817:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD22	1:A:775:ILE:HG21	1.91	0.52
1:A:214:ILE:HD12	1:A:214:ILE:N	2.26	0.51
1:A:679:VAL:HG12	1:A:680:GLU:O	2.11	0.51
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.40	0.51
1:A:289:ILE:O	1:A:293:ILE:HG13	2.10	0.51
1:A:541:VAL:O	1:A:545:ILE:HG12	2.10	0.51
1:A:743:ILE:O	1:A:747:VAL:HG23	2.11	0.51
1:A:895:GLU:N	1:A:896:PRO:HD2	2.25	0.51
1:A:367:PHE:CE1	1:A:596:VAL:HB	2.45	0.51
1:A:953:LEU:N	1:A:954:PRO:HD2	2.27	0.50
1:A:161:ALA:O	1:A:163:ILE:HG13	2.12	0.50
1:A:310:GLY:O	1:A:314:VAL:HG23	2.10	0.50
1:A:321:LEU:HD13	1:A:809:PHE:CZ	2.46	0.50
1:A:52:LEU:HG	1:A:106:VAL:HG23	1.93	0.50
1:A:757:MET:O	1:A:761:ILE:HG13	2.12	0.50
1:A:979:GLY:O	1:A:983:ILE:HG13	2.12	0.50
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.95	0.49
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.42	0.49
1:A:332:ILE:HB	1:A:734:VAL:HB	1.95	0.49
1:A:384:ILE:N	1:A:384:ILE:HD12	2.26	0.49
1:A:817:MET:HA	1:A:817:MET:HE2	1.95	0.49
1:A:116:ILE:N	1:A:116:ILE:HD12	2.27	0.49
1:A:41:LEU:HD23	1:A:236:ARG:HG3	1.94	0.49
1:A:48:SER:C	1:A:49:LEU:HD12	2.34	0.48
1:A:494:MET:N	1:A:515:LYS:O	2.43	0.48
1:A:454:VAL:HG23	1:A:455:PHE:CD2	2.48	0.48
1:A:535:VAL:HB	1:A:536:PRO:HD2	1.96	0.47
1:A:385:THR:HG23	1:A:396:LEU:HD21	1.96	0.47
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.96	0.47
1:A:887:ASP:OD1	1:A:888:CYS:N	2.48	0.47
1:A:43:ALA:O	1:A:45:GLU:N	2.48	0.47
1:A:150:ILE:HG23	1:A:220:LEU:HD21	1.96	0.47
1:A:368:ILE:HD12	1:A:409:GLY:HA3	1.97	0.46
1:A:604:ARG:HB3	1:A:607:VAL:HG13	1.96	0.46
1:A:631:THR:O	1:A:635:ILE:HG13	2.16	0.46
1:A:683:HIS:O	1:A:687:ILE:HG13	2.15	0.46
1:A:907:ILE:HG23	1:A:977:VAL:HG11	1.97	0.46
1:A:369:ILE:HD13	1:A:379:LEU:CD2	2.45	0.46
1:A:817:MET:CE	1:A:817:MET:HA	2.45	0.46
1:A:787:LEU:HD13	1:A:792:LEU:HD21	1.98	0.45
1:A:865:VAL:HG12	1:A:866:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:ALA:HB2	1:A:903:VAL:HG21	1.99	0.45
1:A:334:ARG:HG3	1:A:731:SER:O	2.16	0.45
1:A:604:ARG:O	1:A:607:VAL:HG22	2.16	0.45
1:A:315:ILE:O	1:A:319:LEU:HD13	2.17	0.45
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.98	0.45
1:A:983:ILE:O	1:A:987:ILE:HG13	2.16	0.45
1:A:231:GLU:O	1:A:235:ILE:HG13	2.17	0.45
1:A:350:SER:HA	1:A:701:THR:HG22	1.98	0.45
1:A:802:LEU:N	1:A:803:PRO:HD2	2.32	0.45
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.89	0.44
1:A:604:ARG:HB2	1:A:607:VAL:HG13	1.99	0.44
1:A:413:LEU:HD22	1:A:564:LEU:HD12	2.00	0.44
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.99	0.44
1:A:923:MET:HG3	5:A:1005:PTY:C11	2.48	0.44
1:A:687:ILE:O	1:A:691:LEU:HD13	2.18	0.44
1:A:950:VAL:O	1:A:954:PRO:HD2	2.18	0.44
1:A:811:PRO:HG2	1:A:929:VAL:HG11	2.00	0.43
1:A:93:VAL:HG12	1:A:793:LEU:HD13	2.01	0.43
1:A:933:LEU:O	1:A:937:ILE:HG13	2.18	0.43
1:A:798:VAL:O	1:A:802:LEU:HD23	2.18	0.43
1:A:720:MET:HE3	1:A:738:ASP:CB	2.49	0.43
1:A:975:LEU:N	1:A:976:PRO:CD	2.81	0.43
1:A:767:SER:O	1:A:771:GLU:HG3	2.19	0.43
1:A:61:LEU:HD11	1:A:260:LEU:HD23	2.01	0.43
1:A:321:LEU:HD13	1:A:809:PHE:HZ	1.82	0.43
1:A:402:ILE:HD12	1:A:402:ILE:C	2.39	0.43
1:A:926:PRO:O	1:A:929:VAL:HG23	2.19	0.43
1:A:71:ILE:O	1:A:75:LEU:HD13	2.19	0.42
1:A:880:HIS:N	1:A:881:PRO:CD	2.82	0.42
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.38	0.42
1:A:365:LYS:HE3	1:A:552:TRP:CE2	2.54	0.42
1:A:974:SER:O	1:A:977:VAL:HG12	2.20	0.42
1:A:25:THR:HG23	1:A:28:GLN:H	1.84	0.42
1:A:518:PRO:O	1:A:522:ILE:HG12	2.20	0.42
1:A:765:ILE:O	1:A:769:VAL:HG23	2.20	0.42
1:A:19:SER:HB3	1:A:22:THR:OG1	2.20	0.42
1:A:250:GLN:HG2	4:A:1004:7BS:H51	2.00	0.42
1:A:545:ILE:O	1:A:549:ILE:HG13	2.19	0.42
1:A:3:ALA:O	1:A:7:LYS:HG2	2.20	0.42
1:A:604:ARG:HB2	1:A:607:VAL:CG1	2.50	0.42
1:A:502:LYS:HB3	1:A:502:LYS:NZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.50	0.41
1:A:71:ILE:HG23	1:A:296:PHE:CD2	2.55	0.41
1:A:179:ILE:H	1:A:179:ILE:CD1	2.29	0.41
1:A:549:ILE:HD11	1:A:596:VAL:HG21	2.03	0.41
1:A:41:LEU:HA	1:A:42:PRO:HD3	1.93	0.41
1:A:103:ILE:O	1:A:106:VAL:HG12	2.20	0.41
1:A:214:ILE:HD12	1:A:214:ILE:H	1.85	0.41
1:A:581:SER:HA	1:A:584:PHE:CE1	2.56	0.41
1:A:23:GLY:HA3	1:A:130:TYR:O	2.20	0.41
1:A:315:ILE:HD11	4:A:1004:7BS:C4	2.50	0.41
1:A:481:LYS:HE2	1:A:484:THR:CG2	2.51	0.41
1:A:1:AME:HA	1:A:1:AME:HT23	1.08	0.41
1:A:96:LEU:C	1:A:96:LEU:HD23	2.42	0.41
1:A:97:ILE:HD11	1:A:797:LEU:CD2	2.48	0.41
1:A:220:LEU:C	1:A:220:LEU:HD23	2.40	0.41
1:A:236:ARG:C	1:A:236:ARG:HD3	2.42	0.41
1:A:534:ARG:HG2	1:A:535:VAL:N	2.36	0.41
1:A:571:PRO:HG2	1:A:576:MET:SD	2.61	0.41
1:A:791:GLN:O	1:A:795:VAL:HG23	2.21	0.41
1:A:49:LEU:HD12	1:A:49:LEU:N	2.36	0.41
1:A:567:ARG:HD3	1:A:570:PRO:HA	2.02	0.41
1:A:627:ASP:O	1:A:677:ALA:HB1	2.20	0.41
1:A:810:ASN:HA	1:A:811:PRO:HD3	1.98	0.41
1:A:65:LEU:HB3	1:A:98:LEU:HD21	2.03	0.40
1:A:266:LEU:C	1:A:266:LEU:HD13	2.41	0.40
1:A:485:LEU:HD22	1:A:584:PHE:CE2	2.55	0.40
1:A:901:LEU:HD13	1:A:959:LEU:HD11	2.02	0.40
1:A:260:LEU:O	1:A:264:ILE:HG13	2.21	0.40
1:A:319:LEU:HD11	1:A:757:MET:HE2	2.02	0.40
1:A:917:SER:OG	1:A:920:GLN:HB2	2.21	0.40
1:A:680:GLU:HB2	1:A:683:HIS:CD2	2.57	0.40
1:A:470:ALA:O	1:A:474:VAL:HG23	2.21	0.40
1:A:90:GLU:O	1:A:94:ILE:HG13	2.21	0.40
1:A:161:ALA:HA	1:A:210:SER:HB2	2.03	0.40
1:A:953:LEU:H	1:A:954:PRO:HD2	1.87	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	992/994 (100%)	927 (93%)	62 (6%)	3 (0%)	37 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	885	GLY
1	A	992	LEU

### 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	839/839 (100%)	828 (99%)	11 (1%)	65 83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	179	ILE
1	A	198	ARG
1	A	371	LYS
1	A	396	LEU
1	A	529	ARG
1	A	604	ARG
1	A	613	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	656	ARG
1	A	816	ILE
1	A	886	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	683	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	AME	A	1	1	9,10,11	1.43	2 (22%)	9,11,13	1.91	4 (44%)

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
1	AME	A	1	1	-	4/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	AME	CA-N	3.12	1.50	1.46
1	A	1	AME	CT1-N	-2.81	1.24	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	AME	CA-N-CT1	-3.74	116.25	123.15
1	A	1	AME	O-C-CA	-2.18	119.08	124.78
1	A	1	AME	C-CA-N	2.17	113.66	109.73
1	A	1	AME	OT-CT1-N	2.17	125.94	121.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	AME	O-C-CA-CB
1	A	1	AME	CT2-CT1-N-CA
1	A	1	AME	OT-CT1-N-CA
1	A	1	AME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	AME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
5	PTY	A	1005	-	18,18,49	1.35	3 (16%)	21,23,54	1.12	2 (9%)
4	7BS	A	1004	-	43,44,44	0.82	0	47,57,57	1.78	6 (12%)
5	PTY	A	1006	-	18,18,49	1.25	3 (16%)	21,23,54	1.01	1 (4%)
3	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.04	0

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
5	PTY	A	1005	-	-	7/20/20/53	-
5	PTY	A	1006	-	-	6/20/20/53	-
4	7BS	A	1004	-	-	12/49/69/69	0/1/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	PTY	P1-O13	2.99	1.61	1.50
5	A	1005	PTY	C1-C6	2.97	1.59	1.50
5	A	1006	PTY	C1-C6	2.84	1.59	1.50
5	A	1006	PTY	P1-O13	2.20	1.58	1.50
5	A	1005	PTY	C5-C6	2.17	1.57	1.50
5	A	1006	PTY	C5-C6	2.09	1.57	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1004	7BS	C33-O29-C24	8.53	129.72	115.63
4	A	1004	7BS	C2-C1-C4	3.43	130.23	121.02
4	A	1004	7BS	O71-C31-C30	-3.35	102.27	110.29
5	A	1005	PTY	O4-C1-C6	2.84	116.71	108.43
5	A	1006	PTY	O7-C8-C11	2.71	116.08	111.09
5	A	1005	PTY	O7-C8-C11	2.67	116.01	111.09
4	A	1004	7BS	C3-C1-C4	-2.63	118.57	123.78
4	A	1004	7BS	C8-C4-C1	2.43	131.18	126.50
4	A	1004	7BS	C20-C21-C22	2.02	119.01	112.69

There are no chirality outliers.



All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	7BS	O67-C20-C21-C22
4	A	1004	7BS	C17-C20-C21-C22
4	A	1004	7BS	C22-C23-C24-C27
4	A	1004	7BS	C23-C24-C27-C26
5	A	1005	PTY	C11-C8-O7-C6
5	A	1005	PTY	C3-O11-P1-O14
4	A	1004	7BS	O34-C33-O29-C24
5	A	1006	PTY	C11-C8-O7-C6
4	A	1004	7BS	C32-C33-O29-C24
5	A	1005	PTY	C31-C30-O4-C1
5	A	1005	PTY	O10-C8-O7-C6
5	A	1006	PTY	O10-C8-O7-C6
5	A	1006	PTY	O30-C30-O4-C1
5	A	1005	PTY	O30-C30-O4-C1
5	A	1006	PTY	C31-C30-O4-C1
5	A	1005	PTY	N1-C2-C3-O11
4	A	1004	7BS	O29-C24-C27-C26
4	A	1004	7BS	C20-C21-C22-C23
5	A	1006	PTY	C3-O11-P1-O14
4	A	1004	7BS	C1-C4-C8-C9
4	A	1004	7BS	C22-C23-C24-O29
4	A	1004	7BS	C27-C24-O29-C33
4	A	1004	7BS	C21-C22-C23-C24
5	A	1006	PTY	C5-O14-P1-O13
5	A	1005	PTY	C2-C3-O11-P1

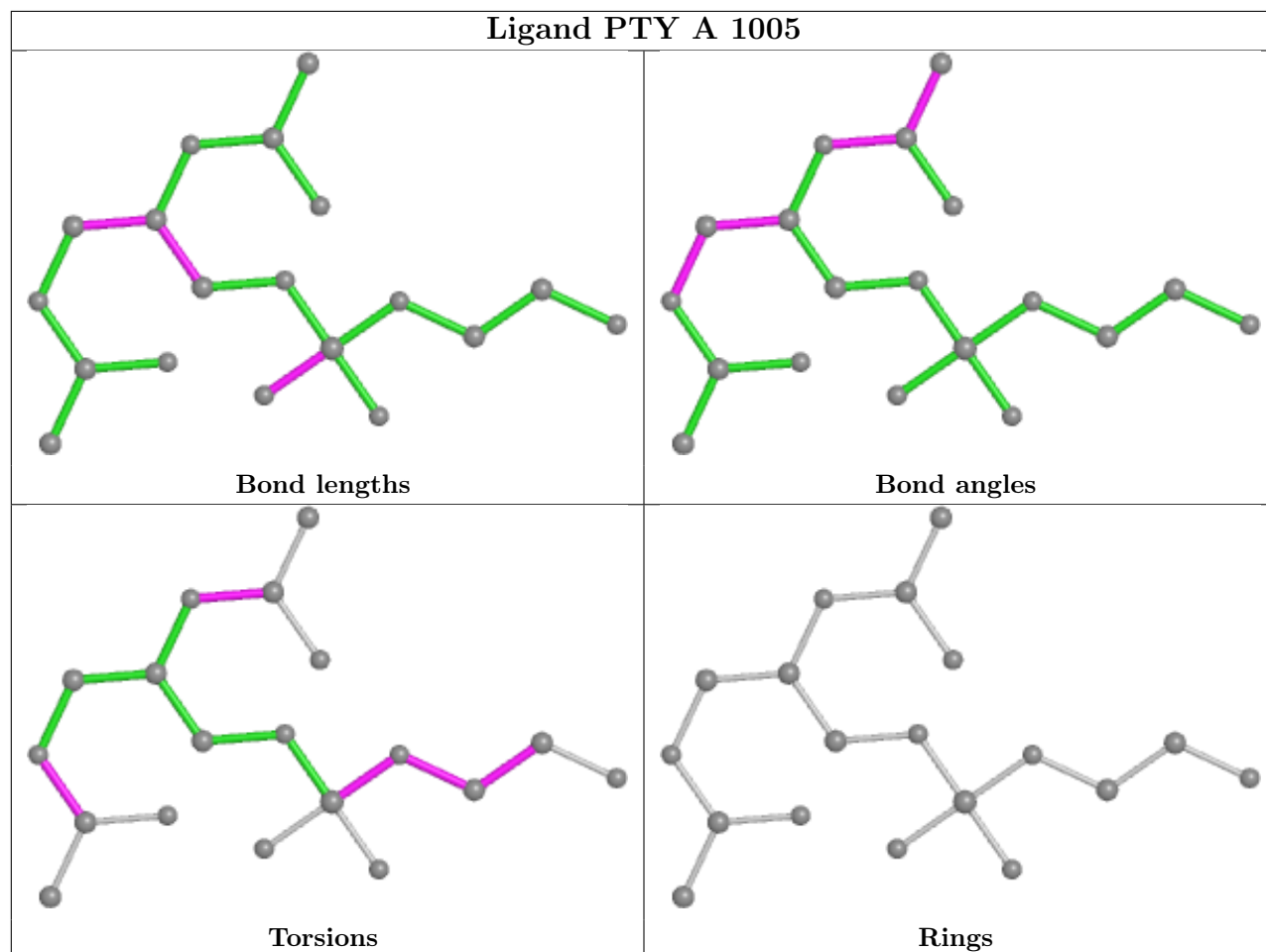
There are no ring outliers.

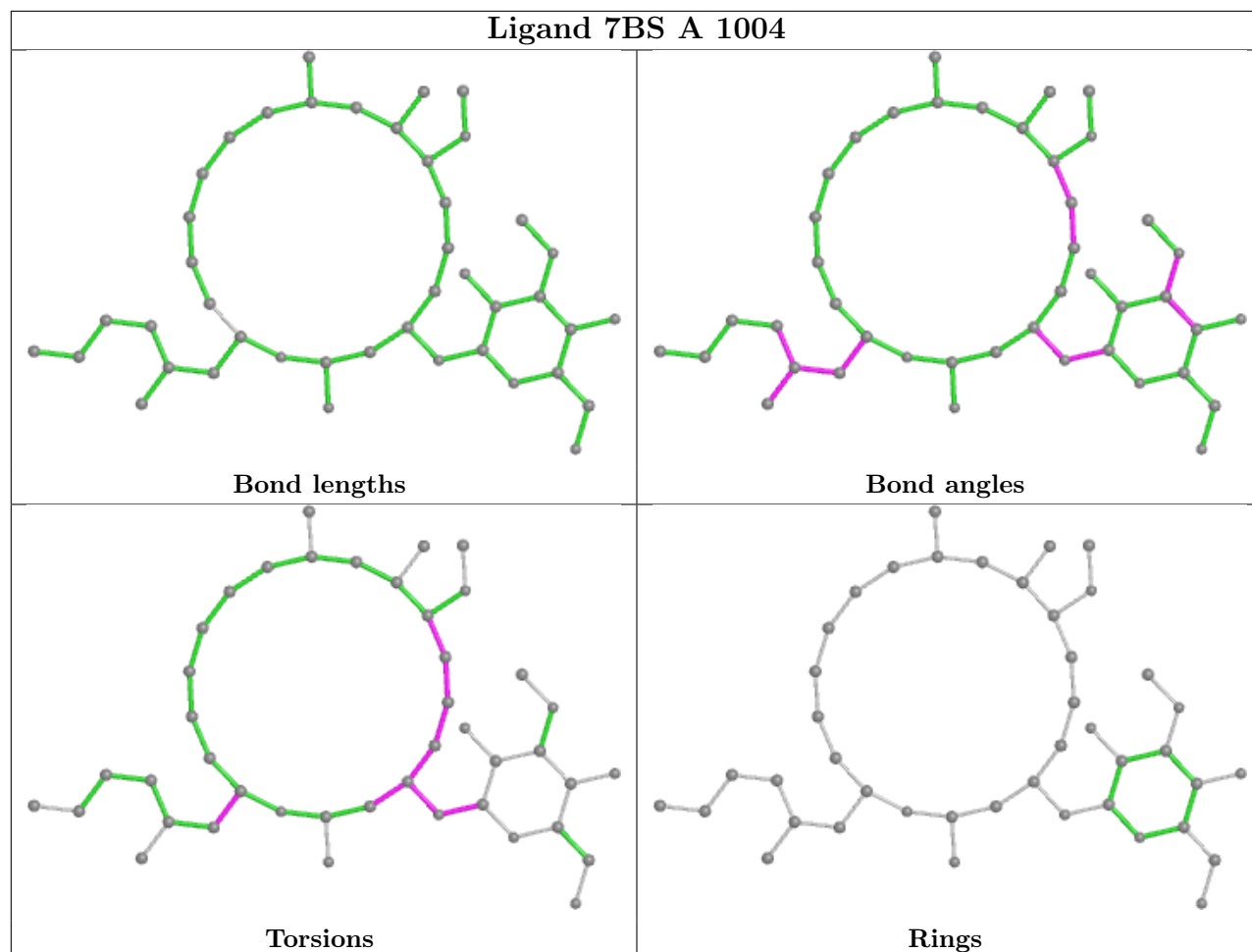
2 monomers are involved in 4 short contacts:

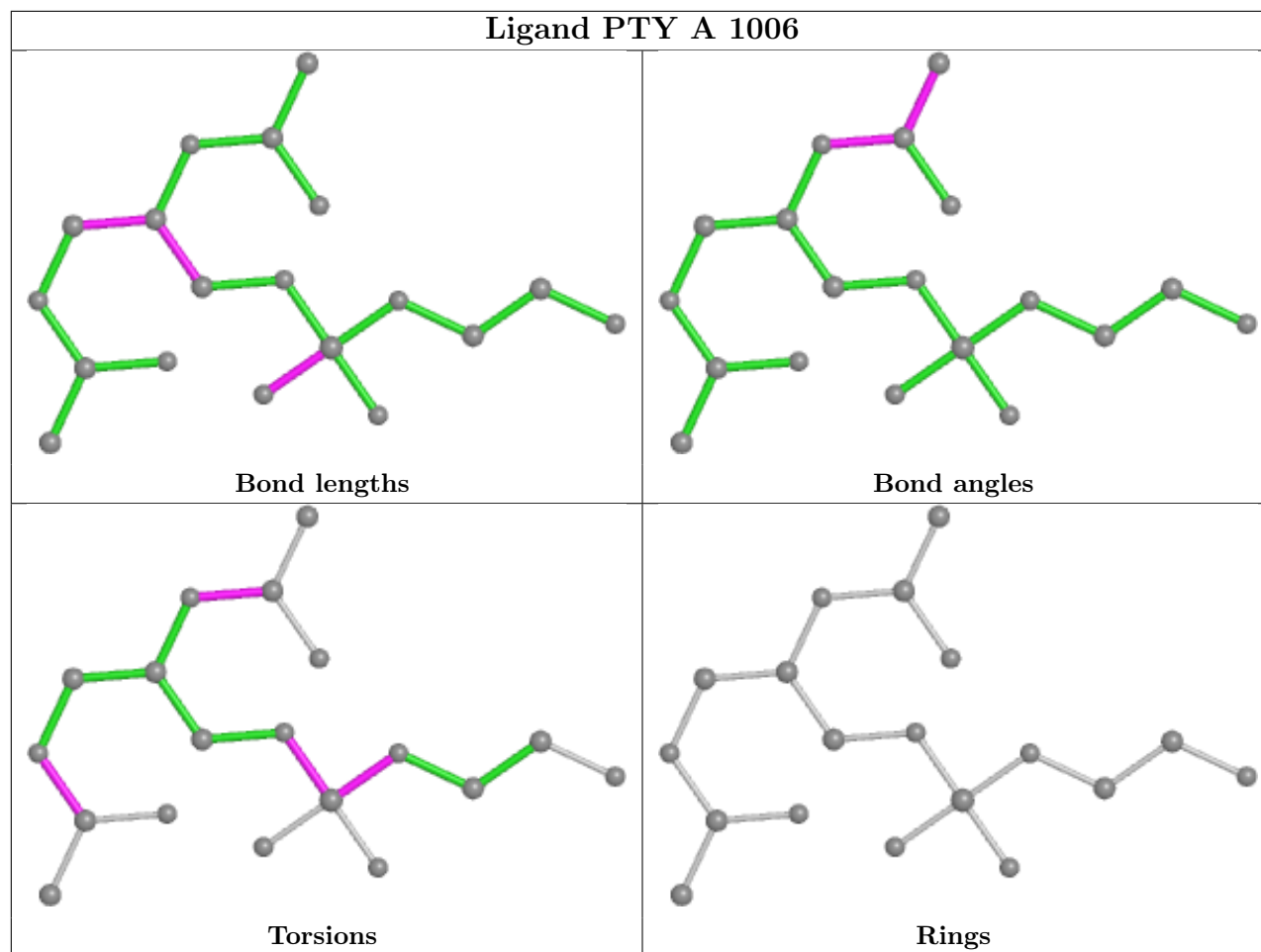
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	PTY	1	0
4	A	1004	7BS	3	0

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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	993/994 (99%)	-0.52	5 (0%) 87 78	33, 78, 163, 296	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ASN	2.4
1	A	112	ALA	2.3
1	A	890	ILE	2.1
1	A	508	VAL	2.1
1	A	48	SER	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	AME	A	1	11/12	0.92	0.10	28,41,85,85	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

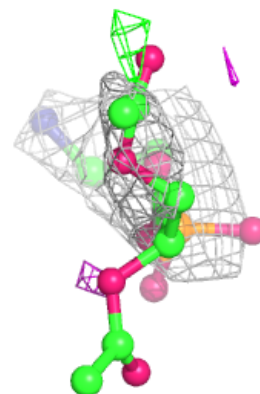
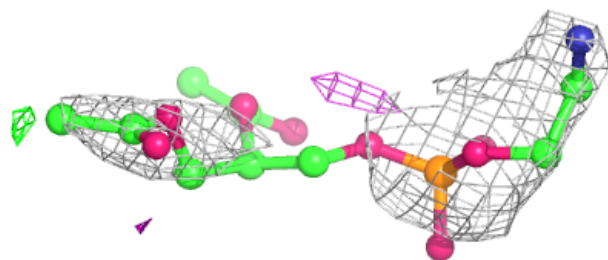
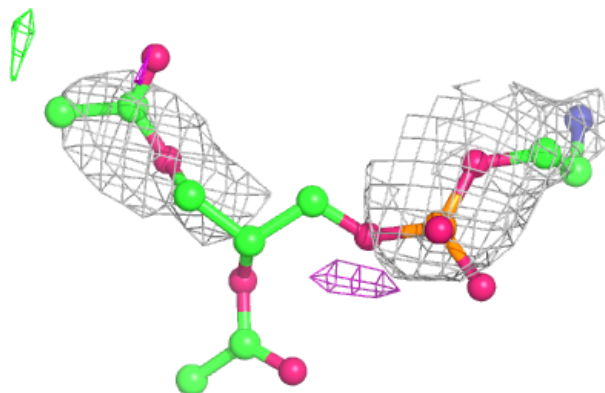
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PTY	A	1005	19/50	0.61	0.14	81,108,166,225	0
5	PTY	A	1006	19/50	0.70	0.12	74,104,164,210	0
2	NA	A	1001	1/1	0.85	0.08	97,97,97,97	0
3	SO4	A	1003	5/5	0.87	0.08	106,109,109,110	0
4	7BS	A	1004	43/43	0.89	0.10	61,85,119,143	0
3	SO4	A	1002	5/5	0.90	0.12	80,81,85,91	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.

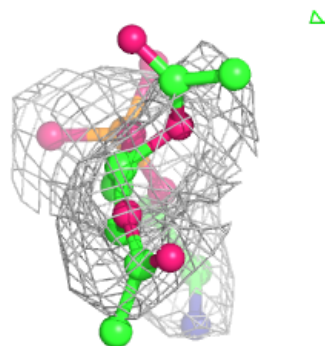
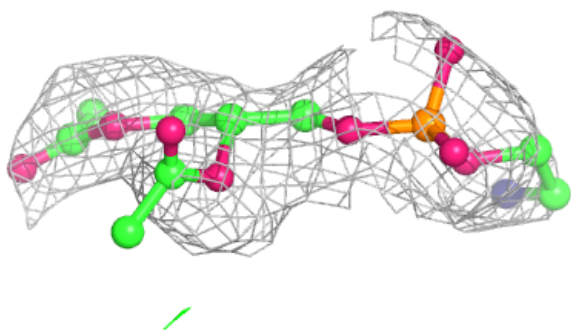
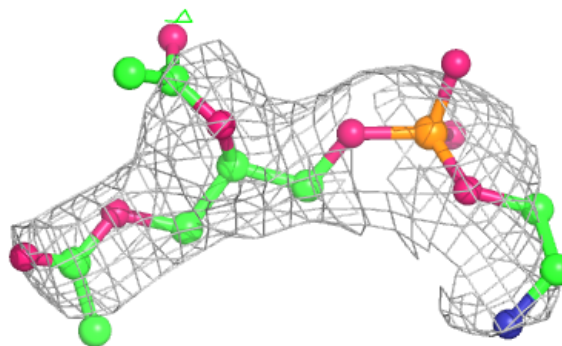
**Electron density around PTY A 1005:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



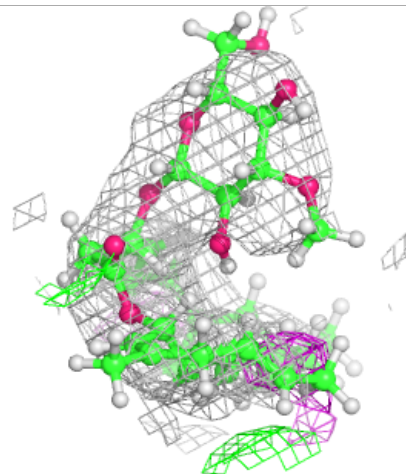
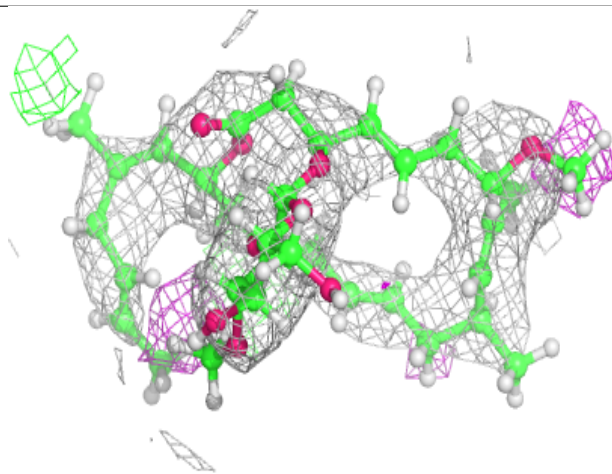
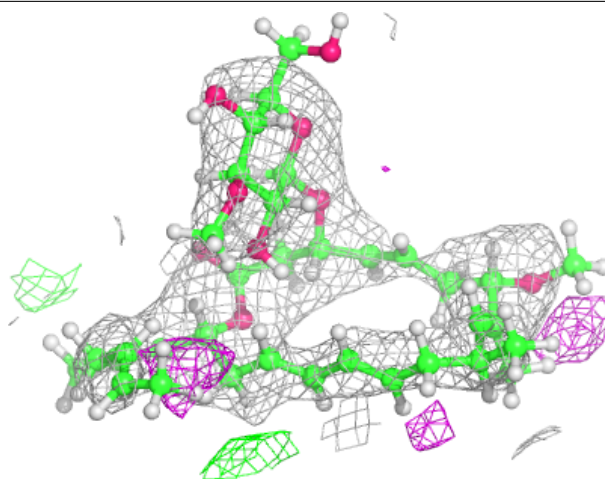
**Electron density around PTY A 1006:**

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



**Electron density around 7BS A 1004:**

$2mF_o-DF_c$  (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.