



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:11 PM UTC

PDB ID : 3AR5 / pdb_00003ar5
Title : Calcium pump crystal structure with bound TNP-AMP and TG
Authors : Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on : 2010-11-24
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

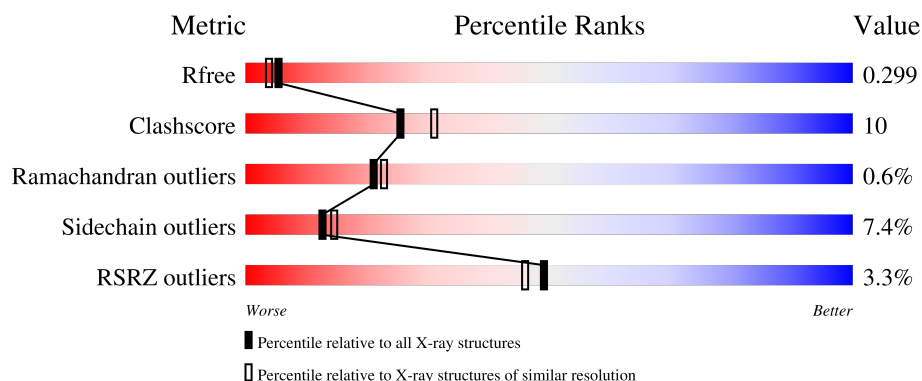
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

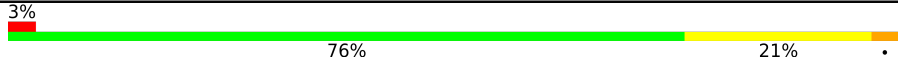
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 ≥ 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	995	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8028 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

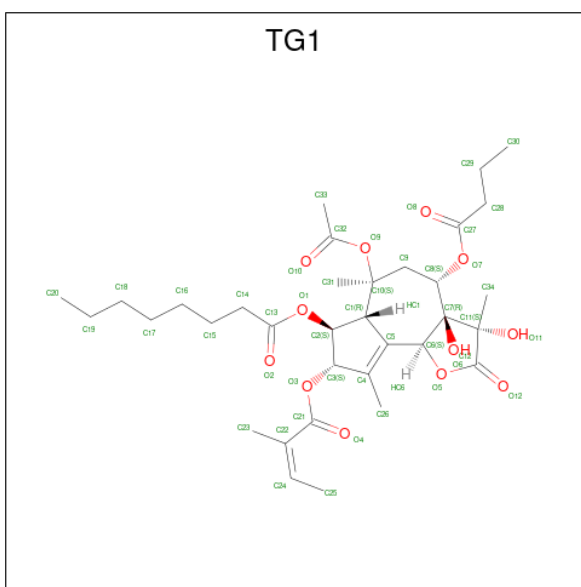
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

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

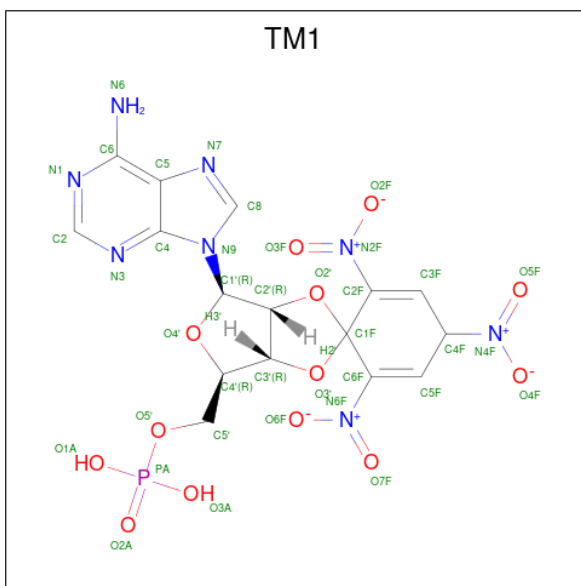
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



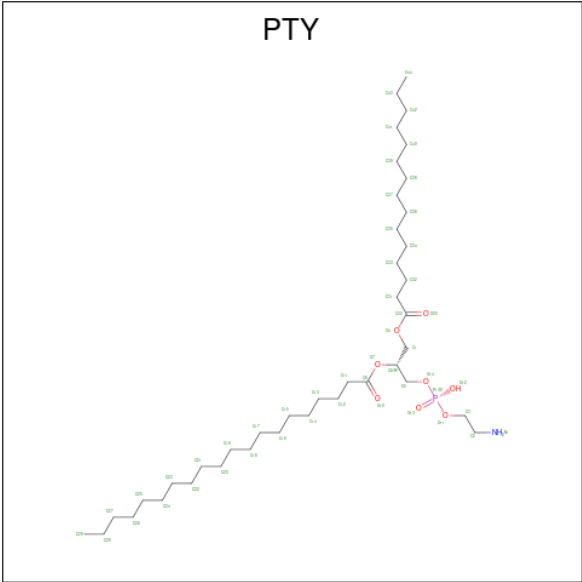
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 4 is 2',3'-O-[(1r)-2,4,6-trinitrocyclohexa-2,5-diene-1,1-diyl]adenosine 5'-(dihydrogen phosphate) (CCD ID: TM1) (formula: $C_{16}H_{15}N_8O_{13}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			38	16	8	13		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

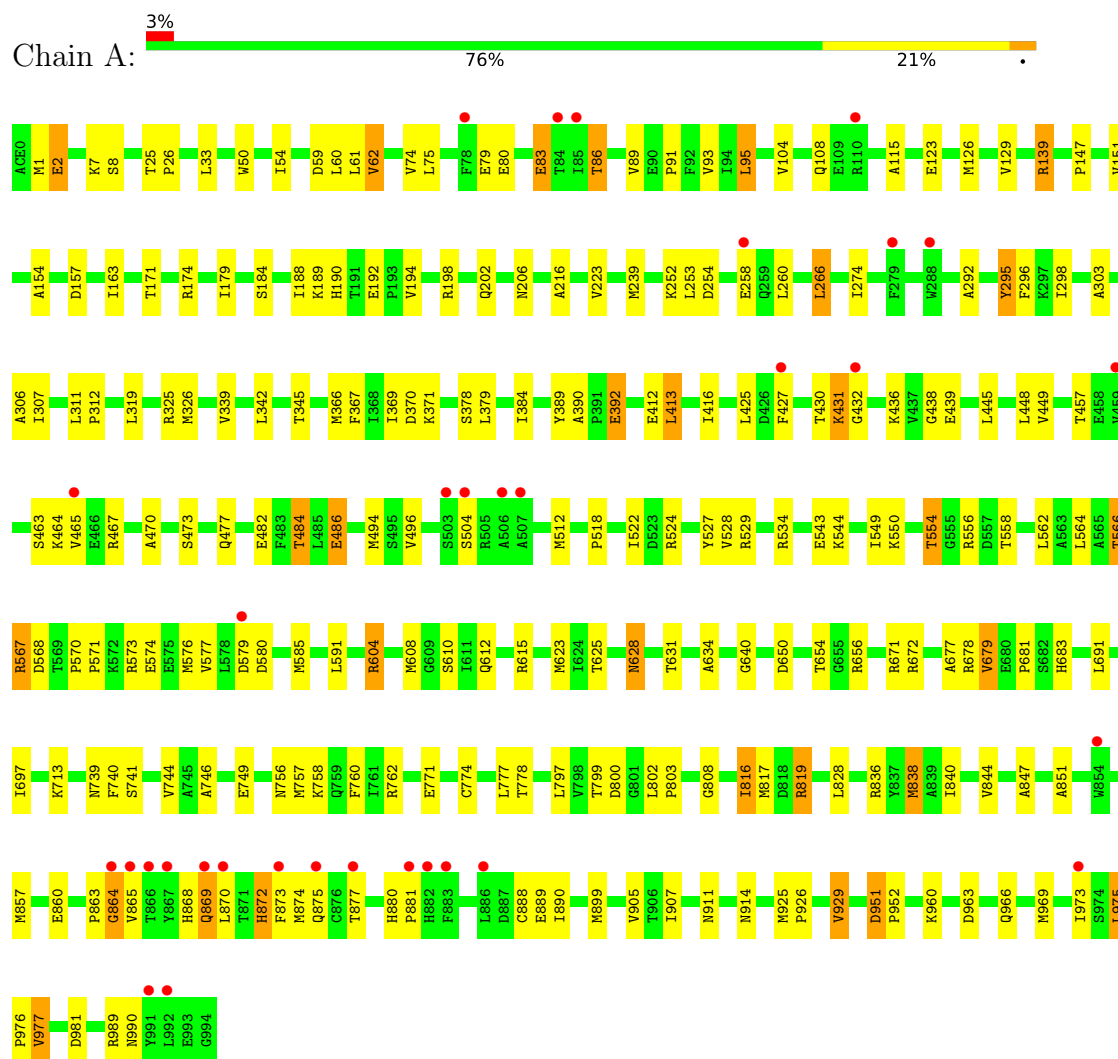
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O	0	0
			212	212		

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, α , β , γ	71.68Å 71.68Å 589.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.20) 99.3 (15.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.20Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, R_{free}	0.260 , 0.288 0.269 , 0.299	Depositor DCC
R_{free} test set	4018 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, TM1, ACE, NA, TG1

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	0.77	1/7813 (0.0%)	0.93	5/10594 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	VAL	N-CA	-5.39	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	874	MET	N-CA-C	-6.54	102.44	110.61
1	A	951	ASP	CA-C-N	-6.39	112.25	119.28
1	A	951	ASP	C-N-CA	-6.39	112.25	119.28
1	A	8	SER	N-CA-C	-5.35	103.63	110.53
1	A	877	THR	N-CA-C	-5.20	106.74	114.64

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	150	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	46	0	50	2	0
4	A	38	0	10	1	0
5	A	57	0	33	3	0
6	A	212	0	0	8	0
All	All	8028	0	7858	150	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 (150) 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:628:ASN:C	1:A:628:ASN:HD22	1.76	0.92
1:A:366:MET:HE1	1:A:448:LEU:HD11	1.57	0.86
1:A:758:LYS:O	1:A:762:ARG:HG3	1.77	0.85
1:A:963:ASP:H	1:A:966:GLN:HE21	1.26	0.84
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.62	0.81
1:A:556:ARG:NH1	6:A:4294:HOH:O	2.14	0.80
1:A:857:MET:O	1:A:864:GLY:HA2	1.80	0.80
1:A:880:HIS:HB2	1:A:881:PRO:HD3	1.66	0.77
1:A:628:ASN:ND2	1:A:631:THR:H	1.82	0.77
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.66	0.76
1:A:615:ARG:NH1	1:A:640:GLY:O	2.19	0.76
1:A:366:MET:CE	1:A:448:LEU:HD11	2.16	0.76
1:A:819:ARG:HG2	1:A:819:ARG:HH11	1.53	0.73
1:A:628:ASN:HD21	1:A:631:THR:H	1.35	0.73
1:A:2:GLU:H	1:A:2:GLU:CD	1.96	0.72
1:A:260:LEU:HD13	3:A:1003:TG1:H252	1.74	0.69
1:A:326:MET:HE1	1:A:339:VAL:HG22	1.75	0.69
1:A:739:ASN:ND2	1:A:741:SER:H	1.92	0.68
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.74	0.68
1:A:254:ASP:O	1:A:258:GLU:HG2	1.94	0.67
1:A:863:PRO:O	1:A:865:VAL:N	2.26	0.67
1:A:83:GLU:HB2	1:A:86:THR:HG22	1.74	0.67
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.96	0.64
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.28	0.63
1:A:366:MET:HE3	1:A:384:ILE:HD11	1.81	0.63
1:A:868:HIS:O	1:A:872:HIS:HD2	1.82	0.63
1:A:838:MET:HE1	3:A:1003:TG1:H141	1.79	0.62
1:A:865:VAL:HB	1:A:868:HIS:CB	2.30	0.62
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:PRO:HG3	1:A:890:ILE:HD13	1.82	0.62
1:A:969:MET:O	1:A:973:ILE:HG22	2.00	0.62
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.82	0.61
1:A:679:VAL:HG22	1:A:683:HIS:ND1	2.15	0.61
1:A:345:THR:HA	1:A:697:ILE:HG22	1.83	0.60
1:A:467:ARG:HH21	1:A:470:ALA:HB3	1.64	0.60
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.83	0.60
1:A:679:VAL:HG22	1:A:683:HIS:CG	2.37	0.59
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.84	0.59
1:A:756:ASN:ND2	1:A:808:GLY:O	2.32	0.59
1:A:800:ASP:C	1:A:803:PRO:HD2	2.28	0.58
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.39	0.57
1:A:427:PHE:HE1	1:A:432:GLY:O	1.88	0.57
1:A:990:ASN:HD21	5:A:1012:PTY:HC31	1.70	0.57
1:A:739:ASN:HD22	1:A:740:PHE:N	2.02	0.57
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.88	0.56
1:A:188:ILE:HD13	1:A:486:GLU:CG	2.35	0.55
1:A:198:ARG:O	1:A:198:ARG:HD3	2.06	0.55
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.88	0.54
1:A:91:PRO:O	1:A:95:LEU:HB2	2.07	0.54
1:A:89:VAL:O	1:A:93:VAL:HG23	2.08	0.54
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.88	0.54
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.90	0.53
1:A:739:ASN:HD22	1:A:741:SER:H	1.55	0.53
1:A:292:ALA:O	1:A:296:PHE:HD1	1.92	0.53
1:A:623:MET:HE3	1:A:625:THR:HG21	1.91	0.53
1:A:963:ASP:H	1:A:966:GLN:NE2	2.00	0.53
1:A:295:TYR:HD1	1:A:295:TYR:N	2.06	0.52
1:A:739:ASN:HD22	1:A:739:ASN:C	2.17	0.52
1:A:757:MET:HA	1:A:760:PHE:CE2	2.44	0.52
1:A:623:MET:HE3	1:A:625:THR:CG2	2.39	0.52
1:A:389:TYR:N	6:A:4239:HOH:O	2.42	0.52
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.45	0.52
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.33	0.51
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.91	0.51
1:A:650:ASP:HB2	1:A:672:ARG:NH1	2.25	0.51
1:A:295:TYR:N	1:A:295:TYR:CD1	2.78	0.51
1:A:473:SER:O	1:A:477:GLN:HG2	2.11	0.51
1:A:869:GLN:OE1	1:A:872:HIS:NE2	2.44	0.51
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.47	0.50
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ARG:CG	1:A:604:ARG:HH11	2.24	0.50
1:A:1:MET:CE	1:A:7:LYS:HG3	2.42	0.50
1:A:550:LYS:O	1:A:554:THR:HB	2.12	0.50
1:A:366:MET:HE3	1:A:384:ILE:CD1	2.42	0.49
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.76	0.49
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.93	0.49
1:A:484:THR:HB	1:A:496:VAL:HG12	1.95	0.49
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.94	0.49
1:A:628:ASN:C	1:A:628:ASN:ND2	2.51	0.49
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.94	0.48
1:A:873:PHE:HD2	1:A:875:GLN:H	1.60	0.48
1:A:369:ILE:HD13	1:A:379:LEU:HD22	1.96	0.48
1:A:427:PHE:CE1	1:A:432:GLY:O	2.65	0.48
1:A:865:VAL:HB	1:A:868:HIS:HB3	1.93	0.48
1:A:126:MET:HE2	1:A:139:ARG:HD3	1.96	0.48
1:A:303:ALA:O	1:A:307:ILE:HG12	2.14	0.48
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.96	0.48
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.61	0.48
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.14	0.47
1:A:25:THR:HB	1:A:26:PRO:HD2	1.96	0.47
1:A:366:MET:HE3	1:A:384:ILE:CG1	2.44	0.47
1:A:872:HIS:HA	6:A:4448:HOH:O	2.14	0.47
1:A:800:ASP:O	1:A:803:PRO:HD2	2.15	0.47
1:A:880:HIS:CB	1:A:881:PRO:HD3	2.40	0.47
1:A:524:ARG:HD3	1:A:585:MET:HE3	1.97	0.46
1:A:926:PRO:O	1:A:929:VAL:HB	2.15	0.46
1:A:543:GLU:OE1	1:A:543:GLU:HA	2.14	0.46
1:A:79:GLU:HG2	1:A:80:GLU:H	1.80	0.46
1:A:571:PRO:HG2	1:A:576:MET:SD	2.56	0.46
1:A:61:LEU:HD13	1:A:307:ILE:HG23	1.98	0.45
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.45
1:A:427:PHE:CZ	1:A:464:LYS:HG2	2.51	0.45
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.98	0.45
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.98	0.45
1:A:819:ARG:HH11	1:A:819:ARG:CG	2.25	0.45
1:A:975:LEU:N	1:A:976:PRO:CD	2.80	0.45
1:A:370:ASP:HB3	1:A:378:SER:OG	2.17	0.45
1:A:681:PRO:HD2	6:A:4328:HOH:O	2.16	0.45
1:A:367:PHE:CD2	1:A:367:PHE:C	2.95	0.45
1:A:838:MET:HA	1:A:838:MET:HE3	1.99	0.45
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.86	0.44
1:A:390:ALA:C	1:A:392:GLU:H	2.25	0.44
1:A:650:ASP:O	1:A:672:ARG:NH1	2.50	0.44
1:A:678:ARG:HD3	4:A:1002:TM1:C6	2.48	0.44
1:A:104:VAL:HG12	1:A:108:GLN:HE21	1.82	0.44
1:A:436:LYS:HE2	1:A:438:GLY:O	2.18	0.44
1:A:179:ILE:HG12	6:A:2101:HOH:O	2.18	0.43
1:A:567:ARG:HG3	1:A:591:LEU:HD23	2.01	0.43
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.00	0.43
1:A:192:GLU:HG2	6:A:2063:HOH:O	2.18	0.43
1:A:851:ALA:HB1	1:A:899:MET:HB3	2.00	0.43
1:A:61:LEU:HD22	1:A:307:ILE:HD12	2.00	0.42
1:A:1:MET:HE1	1:A:7:LYS:HG3	2.00	0.42
1:A:816:ILE:HG22	1:A:817:MET:HG2	2.00	0.42
1:A:654:THR:HA	1:A:677:ALA:O	2.19	0.42
1:A:888:CYS:C	1:A:890:ILE:H	2.28	0.42
1:A:951:ASP:O	1:A:952:PRO:C	2.62	0.42
1:A:713:LYS:HE3	1:A:713:LYS:HB2	1.78	0.42
1:A:59:ASP:HB3	1:A:62:VAL:HG13	2.02	0.42
1:A:604:ARG:CG	1:A:604:ARG:NH1	2.81	0.42
1:A:925:MET:HB3	6:A:4438:HOH:O	2.20	0.42
1:A:482:GLU:OE2	1:A:573:ARG:NH1	2.53	0.42
1:A:771:GLU:O	1:A:774:CYS:HB3	2.19	0.41
1:A:484:THR:HG21	6:A:2038:HOH:O	2.19	0.41
1:A:83:GLU:H	1:A:83:GLU:CD	2.29	0.41
1:A:427:PHE:HD2	1:A:465:VAL:HG22	1.85	0.41
1:A:430:THR:HB	1:A:431:LYS:HD2	2.02	0.41
1:A:989:ARG:NH2	5:A:1012:PTY:HC51	2.35	0.41
1:A:990:ASN:ND2	5:A:1012:PTY:HC31	2.36	0.41
1:A:115:ALA:HB1	1:A:239:MET:HE1	2.03	0.41
1:A:154:ALA:O	1:A:157:ASP:HB2	2.21	0.41
1:A:192:GLU:CD	1:A:580:ASP:HA	2.46	0.41
1:A:836:ARG:O	1:A:840:ILE:HG12	2.20	0.41
1:A:777:LEU:HD23	1:A:777:LEU:HA	1.91	0.41
1:A:190:HIS:O	1:A:206:ASN:HA	2.21	0.41
1:A:252:LYS:HD3	1:A:828:LEU:HD12	2.03	0.41
1:A:311:LEU:HB3	1:A:312:PRO:HD3	2.02	0.40
1:A:907:ILE:HG23	1:A:977:VAL:HG11	2.03	0.40
1:A:366:MET:HE3	1:A:384:ILE:HG12	2.02	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	993/995 (100%)	940 (95%)	47 (5%)	6 (1%)	21 23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	A	864	GLY
1	A	869	GLN
1	A	872	HIS
1	A	463	SER
1	A	889	GLU

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	840/840 (100%)	778 (93%)	62 (7%)	13 14

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	33	LEU
1	A	60	LEU
1	A	62	VAL
1	A	74	VAL

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Mol	Chain	Res	Type
1	A	75	LEU
1	A	83	GLU
1	A	86	THR
1	A	95	LEU
1	A	123	GLU
1	A	139	ARG
1	A	171	THR
1	A	184	SER
1	A	189	LYS
1	A	202	GLN
1	A	253	LEU
1	A	266	LEU
1	A	274	ILE
1	A	295	TYR
1	A	298	ILE
1	A	319	LEU
1	A	371	LYS
1	A	392	GLU
1	A	413	LEU
1	A	425	LEU
1	A	431	LYS
1	A	439	GLU
1	A	445	LEU
1	A	449	VAL
1	A	457	THR
1	A	484	THR
1	A	486	GLU
1	A	494	MET
1	A	522	ILE
1	A	544	LYS
1	A	554	THR
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	577	VAL
1	A	579	ASP
1	A	604	ARG
1	A	608	MET
1	A	612	GLN
1	A	628	ASN
1	A	656	ARG

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Mol	Chain	Res	Type
1	A	671	ARG
1	A	679	VAL
1	A	691	LEU
1	A	778	THR
1	A	797	LEU
1	A	802	LEU
1	A	816	ILE
1	A	819	ARG
1	A	838	MET
1	A	860	GLU
1	A	870	LEU
1	A	929	VAL
1	A	960	LYS
1	A	975	LEU
1	A	977	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	108	GLN
1	A	114	ASN
1	A	202	GLN
1	A	213	ASN
1	A	250	GLN
1	A	510	ASN
1	A	612	GLN
1	A	628	ASN
1	A	739	ASN
1	A	872	HIS
1	A	875	GLN
1	A	911	ASN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN
1	A	990	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
3	TG1	A	1003	-	44,48,48	2.65	9 (20%)	47,72,72	2.35	13 (27%)
5	PTY	A	1011	-	18,18,49	1.56	2 (11%)	21,23,54	1.54	3 (14%)
5	PTY	A	1012	-	18,18,49	1.58	2 (11%)	21,23,54	1.53	3 (14%)
5	PTY	A	1013	-	18,18,49	1.50	2 (11%)	21,23,54	1.39	2 (9%)
4	TM1	A	1002	-	36,42,42	3.19	10 (27%)	43,66,66	2.47	13 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TG1	A	1003	-	-	11/33/99/99	0/3/3/3
5	PTY	A	1011	-	-	10/20/20/53	-
5	PTY	A	1012	-	-	5/20/20/53	-
5	PTY	A	1013	-	-	11/20/20/53	-
4	TM1	A	1002	-	-	5/16/68/68	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	TM1	C5F-C6F	14.39	1.53	1.33
3	A	1003	TG1	O4-C21	11.49	1.44	1.21
3	A	1003	TG1	O5-C12	6.81	1.45	1.35
4	A	1002	TM1	C3'-C4'	-6.49	1.36	1.52
5	A	1011	PTY	O7-C8	5.42	1.47	1.35
4	A	1002	TM1	C4F-C5F	-5.26	1.35	1.50
5	A	1012	PTY	O7-C8	5.12	1.46	1.35
3	A	1003	TG1	C33-C32	-5.06	1.32	1.49
3	A	1003	TG1	O9-C32	5.04	1.46	1.35
5	A	1013	PTY	O7-C8	5.03	1.46	1.35
3	A	1003	TG1	O3-C21	4.73	1.44	1.34
4	A	1002	TM1	O2'-C1F	4.33	1.47	1.41
3	A	1003	TG1	O7-C27	4.05	1.45	1.34
3	A	1003	TG1	O1-C13	4.05	1.45	1.34
5	A	1011	PTY	O4-C30	2.76	1.46	1.33
4	A	1002	TM1	O3'-C1F	2.71	1.45	1.41
5	A	1013	PTY	O4-C30	2.69	1.46	1.33
5	A	1012	PTY	O4-C30	2.62	1.46	1.33
4	A	1002	TM1	C3'-C2'	-2.62	1.47	1.53
4	A	1002	TM1	C5-N7	-2.48	1.34	1.39
4	A	1002	TM1	C3F-C2F	2.42	1.37	1.33
4	A	1002	TM1	C8-N7	2.24	1.36	1.31
3	A	1003	TG1	C9-C8	2.22	1.55	1.52
4	A	1002	TM1	C4-N3	2.12	1.38	1.34
3	A	1003	TG1	O9-C10	-2.03	1.44	1.48

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	TG1	O9-C32-C33	6.90	122.36	110.67
4	A	1002	TM1	O3'-C3'-C4'	6.72	130.51	110.86
3	A	1003	TG1	O3-C21-O4	-6.58	111.12	123.40
3	A	1003	TG1	C6-O5-C12	-5.70	102.89	110.80
3	A	1003	TG1	O4-C21-C22	-5.58	107.58	125.28
4	A	1002	TM1	C5-C4-N3	-5.35	119.36	126.72
5	A	1011	PTY	O7-C8-C11	5.26	120.47	111.09
5	A	1013	PTY	O7-C8-C11	4.82	119.69	111.09
4	A	1002	TM1	O3'-C3'-C2'	4.67	111.08	103.63
4	A	1002	TM1	C5'-C4'-C3'	4.55	129.54	114.38
4	A	1002	TM1	O4'-C4'-C5'	4.49	123.71	109.33
4	A	1002	TM1	N3-C4-N9	4.49	134.79	127.17
4	A	1002	TM1	N3-C2-N1	-4.40	121.92	128.58
4	A	1002	TM1	C2'-C3'-C4'	3.85	112.71	103.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1012	PTY	O7-C8-C11	3.73	117.74	111.09
5	A	1012	PTY	O4-C1-C6	3.64	118.89	108.40
4	A	1002	TM1	C2-N3-C4	3.51	120.41	111.83
3	A	1003	TG1	C10-O9-C32	3.50	129.57	121.36
3	A	1003	TG1	O1-C13-C14	3.21	118.43	111.48
3	A	1003	TG1	O12-C12-C11	-3.14	125.10	128.28
4	A	1002	TM1	N9-C8-N7	-2.96	109.74	113.94
4	A	1002	TM1	O3'-C1F-C6F	-2.84	106.58	110.47
3	A	1003	TG1	O7-C27-C28	2.80	117.55	111.48
4	A	1002	TM1	C4-N9-C8	2.72	108.59	105.74
5	A	1013	PTY	O7-C8-O10	-2.36	118.43	122.99
3	A	1003	TG1	O7-C8-C9	2.34	110.81	106.63
4	A	1002	TM1	O5'-C5'-C4'	2.33	116.92	108.99
3	A	1003	TG1	O1-C2-C3	-2.26	105.92	110.18
3	A	1003	TG1	O9-C32-O10	-2.22	119.74	123.61
5	A	1011	PTY	C1-O4-C30	2.18	122.47	117.08
5	A	1012	PTY	C1-O4-C30	2.14	122.37	117.08
5	A	1011	PTY	O7-C8-O10	-2.14	118.87	122.99
3	A	1003	TG1	C23-C22-C24	-2.12	115.00	123.12
3	A	1003	TG1	C8-O7-C27	-2.11	114.19	118.03

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	TM1	C5'-O5'-PA-O1A
4	A	1002	TM1	C5'-O5'-PA-O3A
5	A	1011	PTY	O4-C1-C6-O7
5	A	1011	PTY	N1-C2-C3-O11
5	A	1011	PTY	C11-C8-O7-C6
5	A	1011	PTY	C3-O11-P1-O13
5	A	1011	PTY	C5-O14-P1-O11
5	A	1011	PTY	C5-O14-P1-O12
5	A	1013	PTY	N1-C2-C3-O11
5	A	1013	PTY	C11-C8-O7-C6
5	A	1013	PTY	C3-O11-P1-O13
5	A	1013	PTY	C5-O14-P1-O13
5	A	1012	PTY	O4-C1-C6-O7
5	A	1012	PTY	C3-O11-P1-O13
5	A	1011	PTY	O10-C8-O7-C6
5	A	1013	PTY	O10-C8-O7-C6
5	A	1011	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
5	A	1011	PTY	O30-C30-O4-C1
5	A	1013	PTY	O30-C30-O4-C1
5	A	1013	PTY	C31-C30-O4-C1
5	A	1012	PTY	C31-C30-O4-C1
4	A	1002	TM1	O4'-C4'-C5'-O5'
5	A	1012	PTY	O30-C30-O4-C1
3	A	1003	TG1	C15-C16-C17-C18
3	A	1003	TG1	C22-C21-O3-C3
5	A	1013	PTY	O14-C5-C6-C1
3	A	1003	TG1	O4-C21-O3-C3
3	A	1003	TG1	C13-C14-C15-C16
5	A	1013	PTY	O4-C1-C6-C5
4	A	1002	TM1	C5'-O5'-PA-O2A
5	A	1012	PTY	O4-C1-C6-C5
5	A	1013	PTY	O14-C5-C6-O7
5	A	1013	PTY	O4-C1-C6-O7
5	A	1011	PTY	O4-C1-C6-C5
3	A	1003	TG1	C16-C17-C18-C19
3	A	1003	TG1	O10-C32-O9-C10
3	A	1003	TG1	C33-C32-O9-C10
4	A	1002	TM1	C5F-C4F-N4F-O5F
3	A	1003	TG1	O1-C13-C14-C15
3	A	1003	TG1	O3-C21-C22-C23
3	A	1003	TG1	O2-C13-C14-C15
3	A	1003	TG1	O7-C27-C28-C29

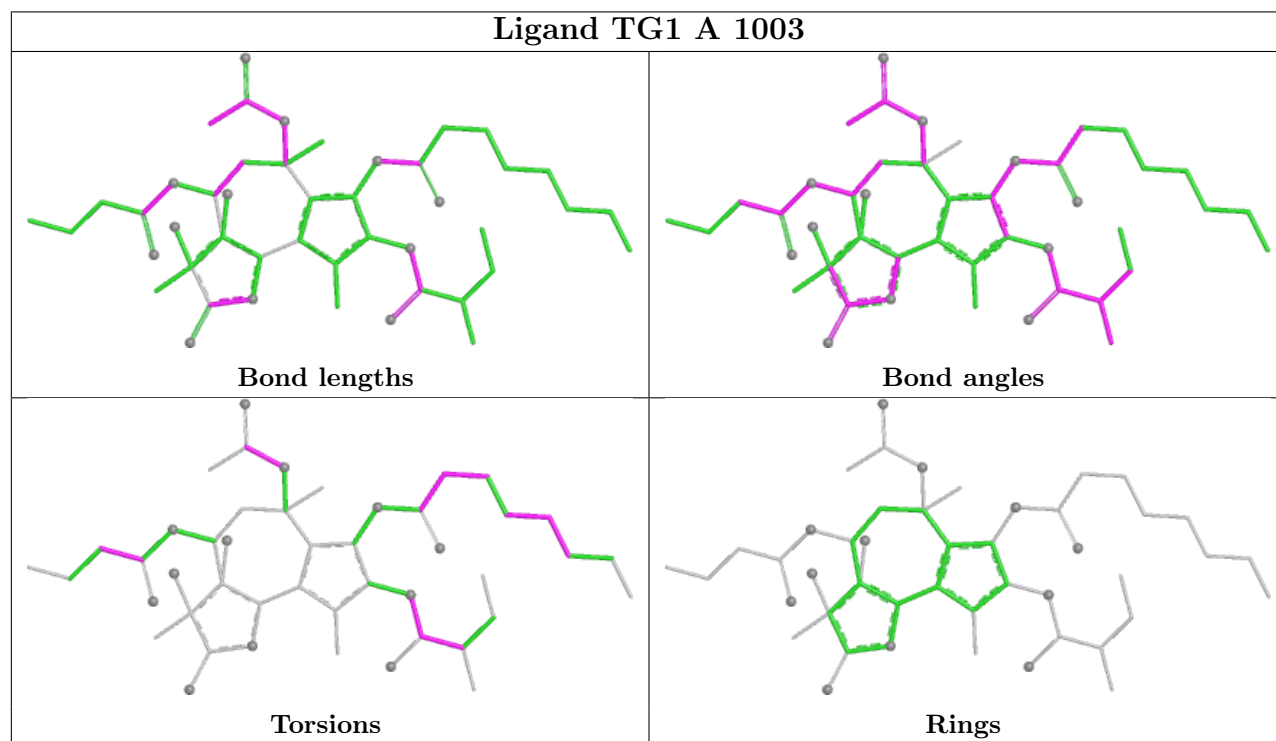
There are no ring outliers.

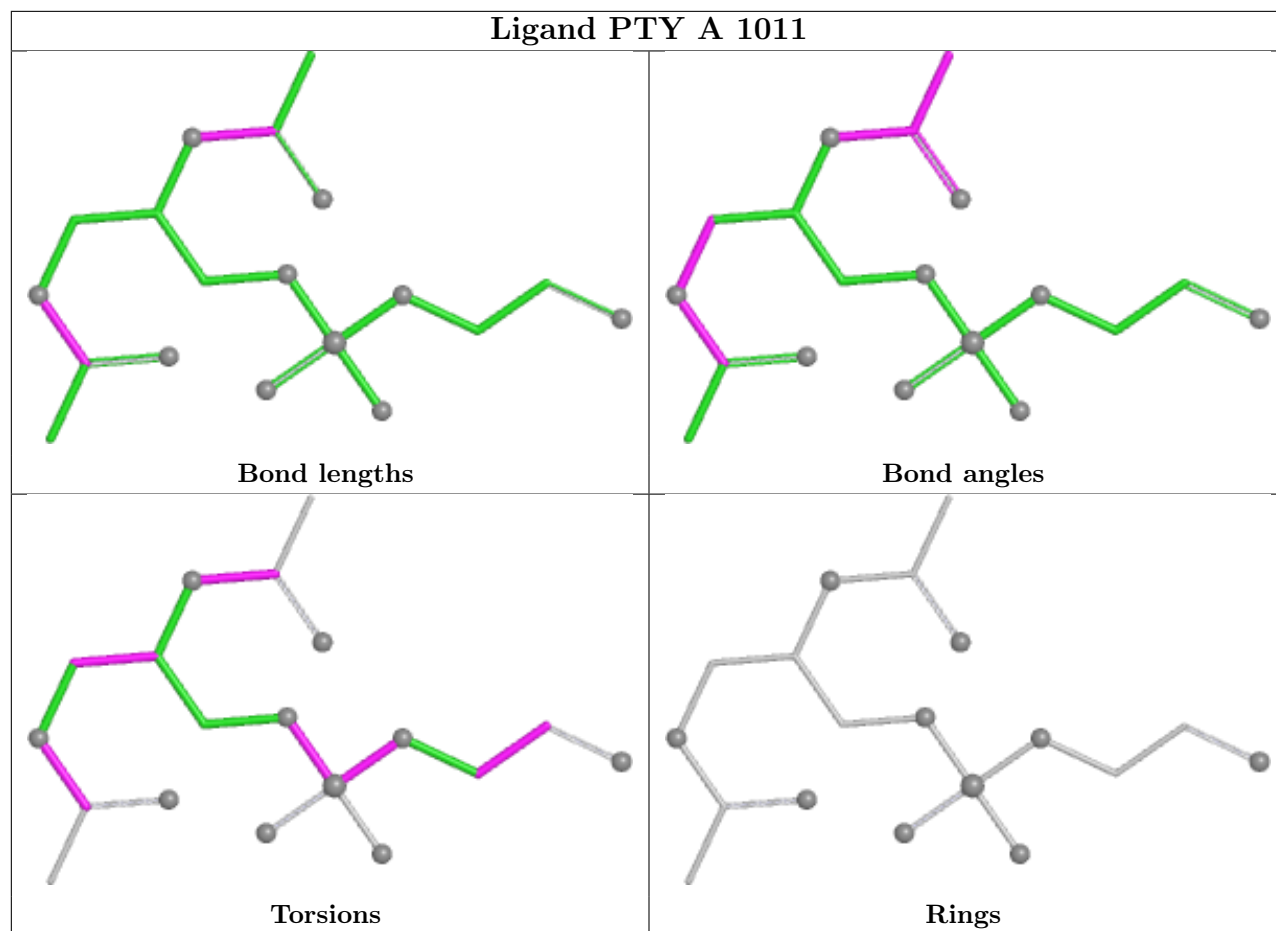
3 monomers are involved in 6 short contacts:

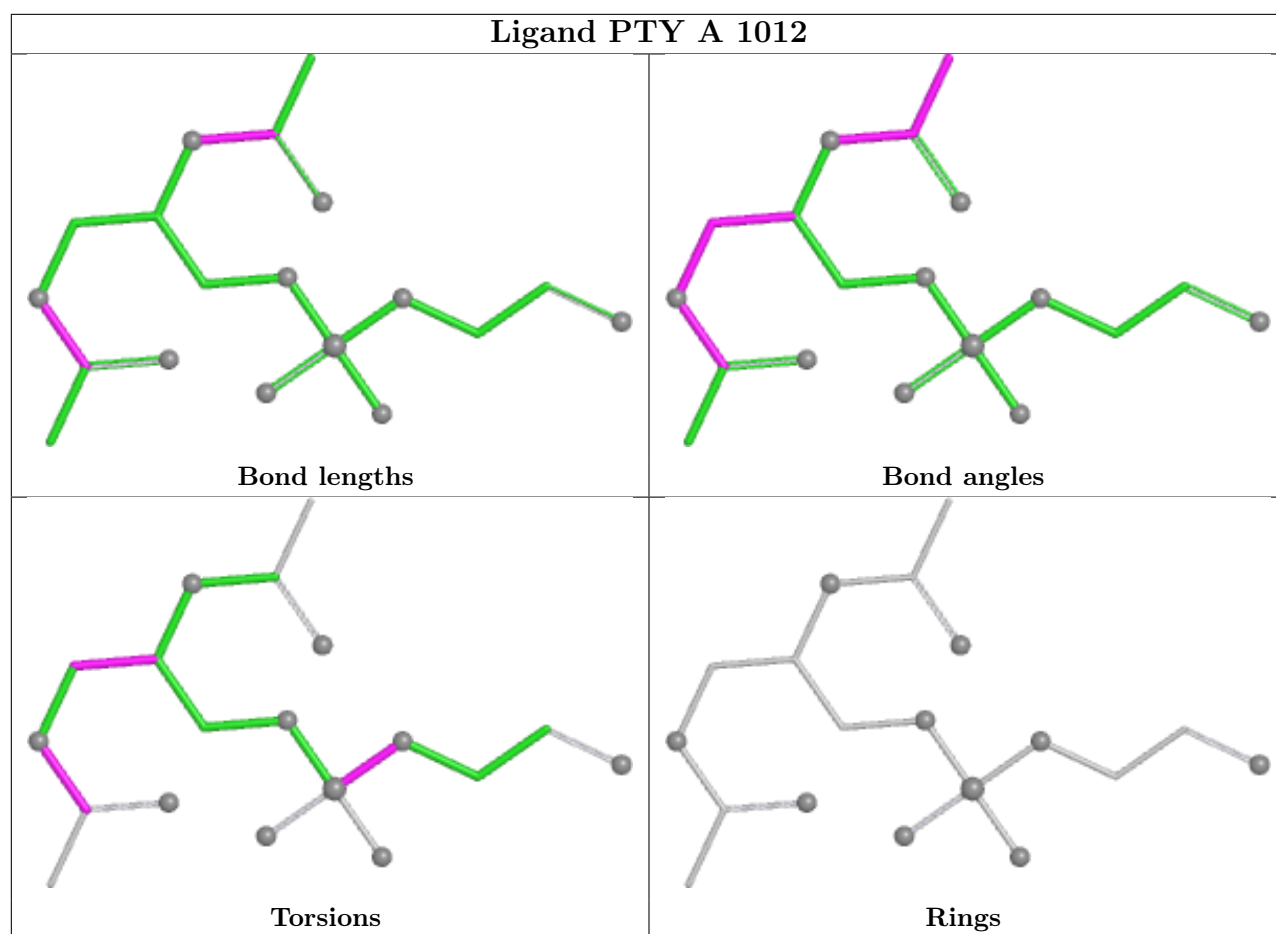
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	TG1	2	0
5	A	1012	PTY	3	0
4	A	1002	TM1	1	0

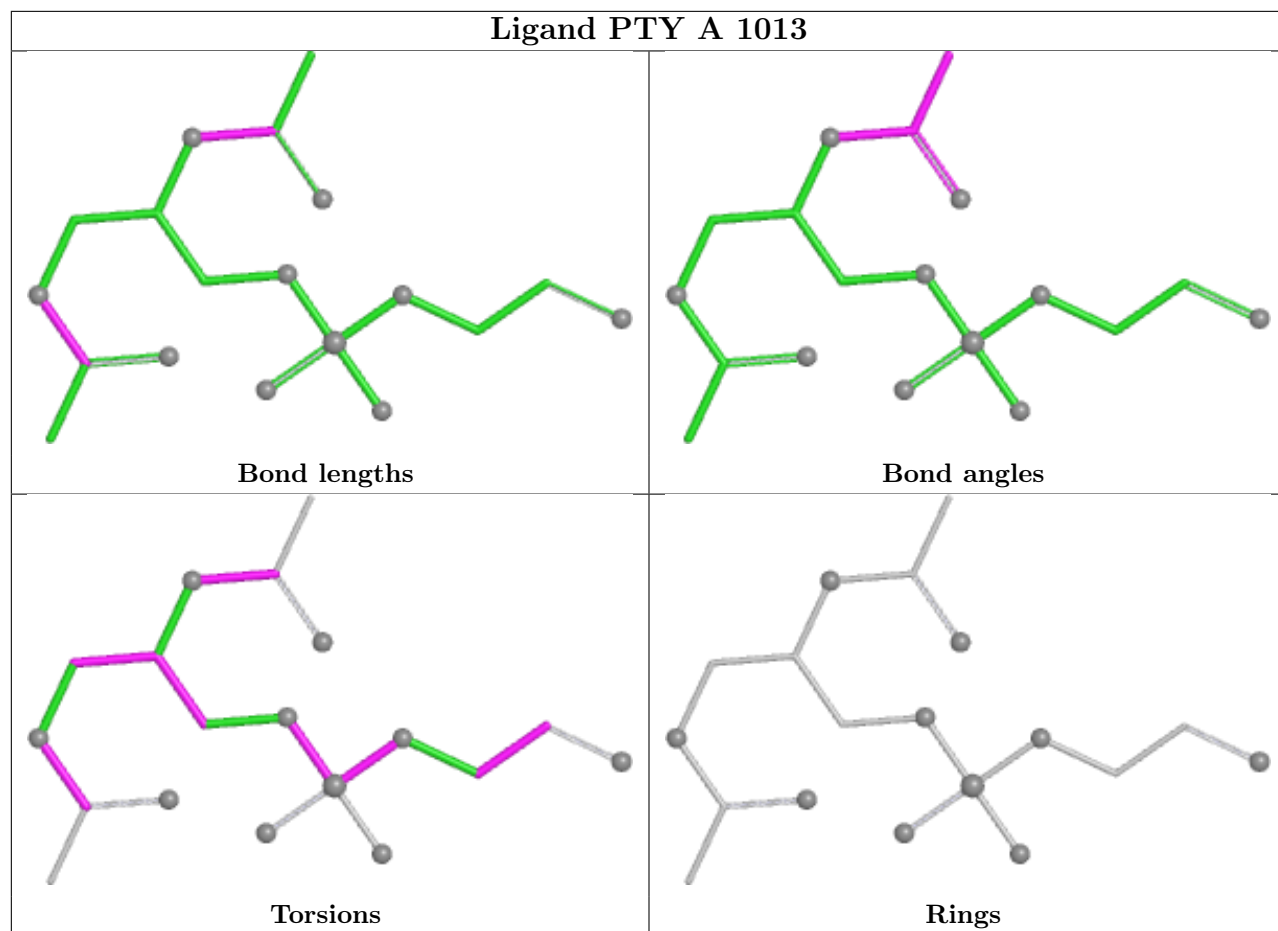
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

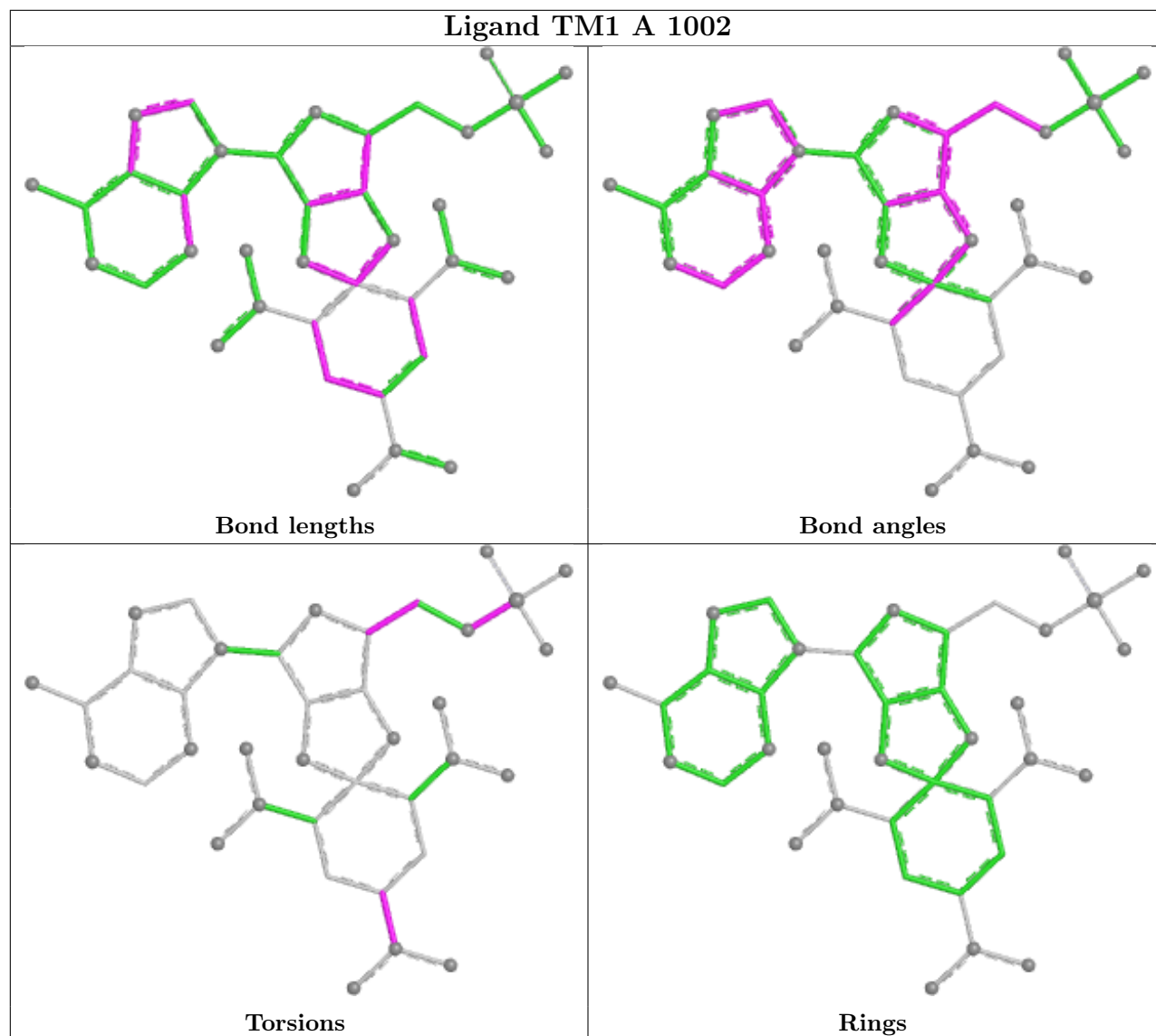
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	994/995 (99%)	0.09	33 (3%)	49 46	35, 65, 121, 155	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	873	PHE	5.6
1	A	883	PHE	5.0
1	A	85	ILE	4.6
1	A	506	ALA	4.5
1	A	886	LEU	4.3
1	A	865	VAL	4.0
1	A	507	ALA	3.7
1	A	866	THR	3.4
1	A	427	PHE	3.3
1	A	78	PHE	3.3
1	A	504	SER	3.3
1	A	875	GLN	3.2
1	A	465	VAL	3.2
1	A	867	TYR	3.1
1	A	579	ASP	3.1
1	A	877	THR	3.0
1	A	84	THR	3.0
1	A	503	SER	2.9
1	A	882	HIS	2.8
1	A	881	PRO	2.7
1	A	432	GLY	2.5
1	A	991	TYR	2.5
1	A	870	LEU	2.4
1	A	992	LEU	2.4
1	A	279	PHE	2.2
1	A	973	ILE	2.2
1	A	110	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLU	2.2
1	A	288	TRP	2.2
1	A	854	TRP	2.1
1	A	869	GLN	2.1
1	A	864	GLY	2.1
1	A	459	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

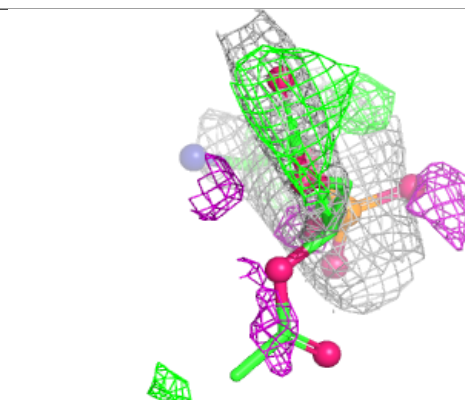
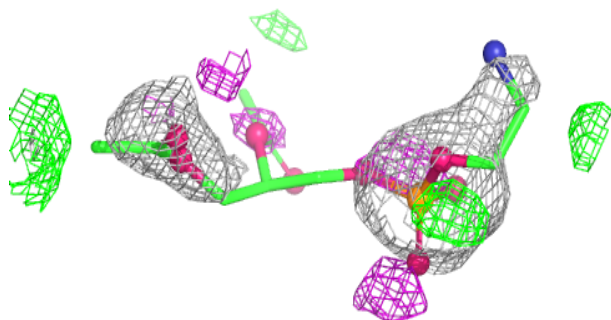
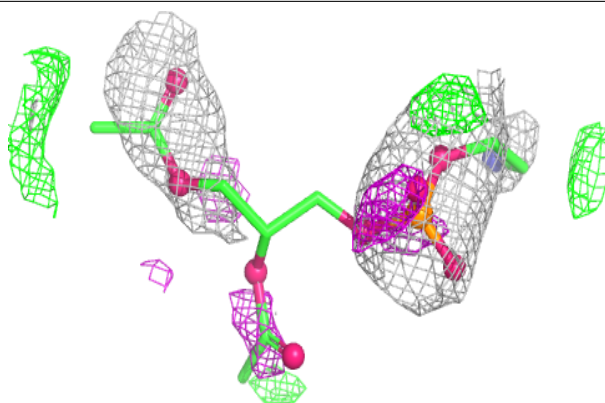
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PTY	A	1012	19/50	0.61	0.18	100,103,106,106	0
5	PTY	A	1013	19/50	0.72	0.14	97,101,103,103	0
5	PTY	A	1011	19/50	0.76	0.17	107,108,110,110	0
3	TG1	A	1003	46/46	0.90	0.09	43,48,62,63	0
4	TM1	A	1002	38/38	0.91	0.08	44,52,70,73	0
2	NA	A	1000	1/1	0.92	0.12	34,34,34,34	0

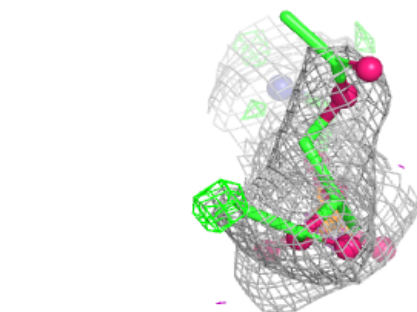
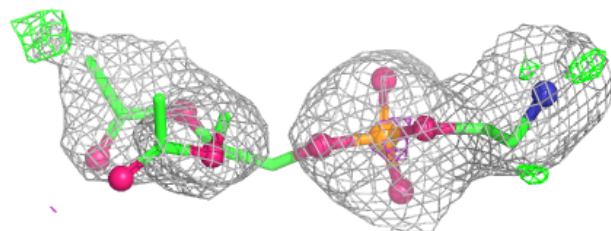
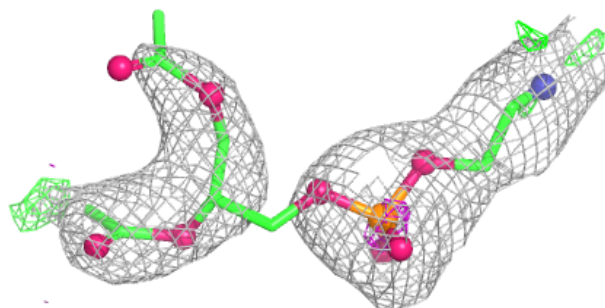
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY A 1012:

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

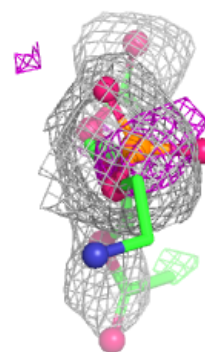
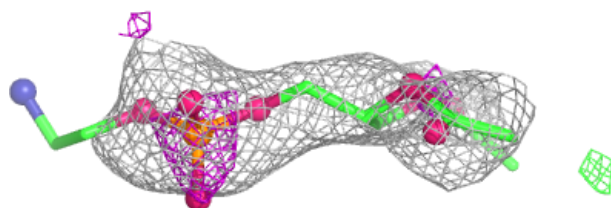
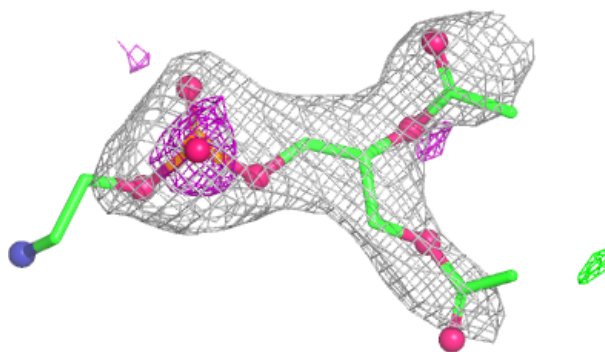
**Electron density around PTY A 1013:**

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

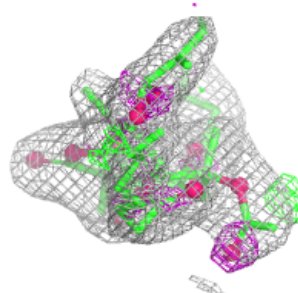
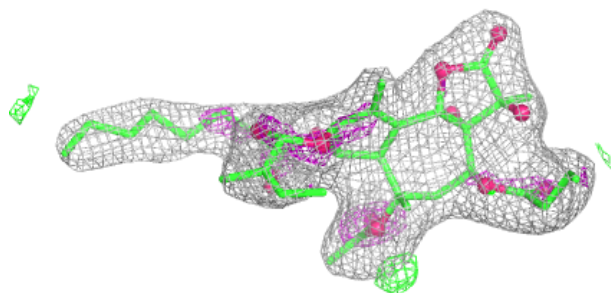
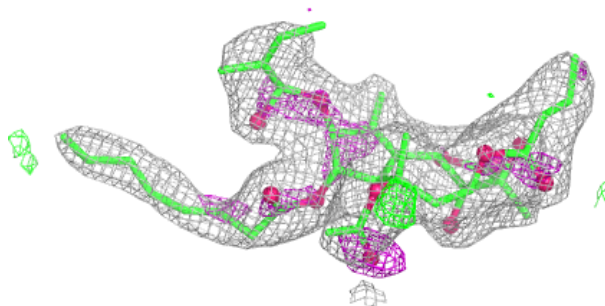


Electron density around PTY A 1011:

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

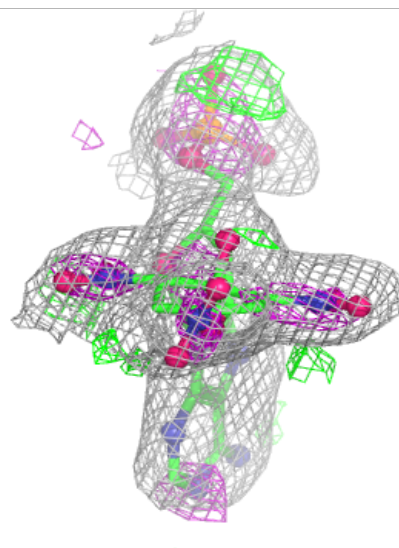
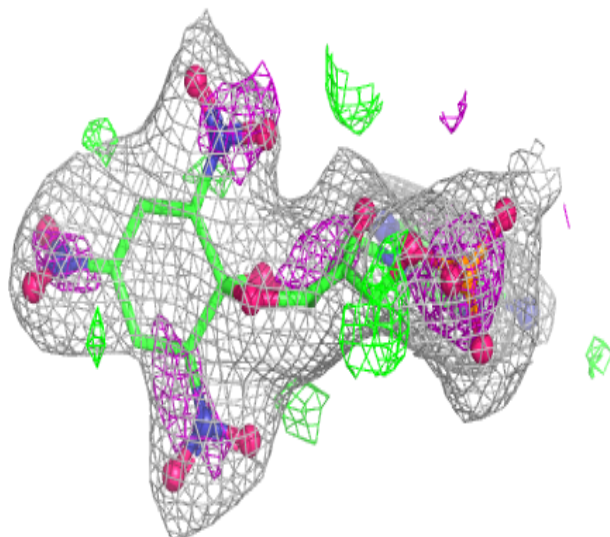
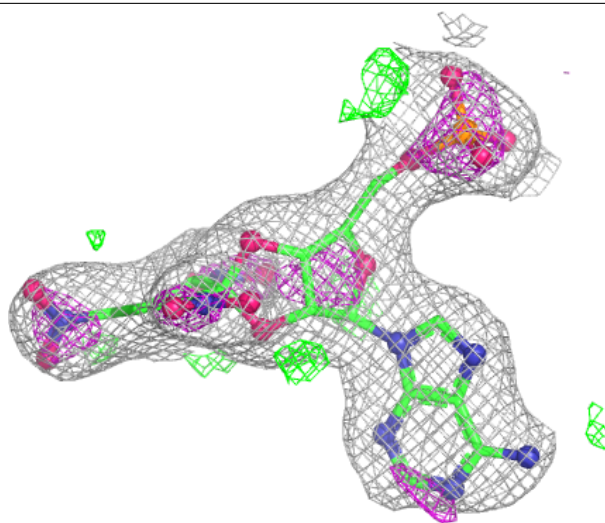
**Electron density around TG1 A 1003:**

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



Electron density around TM1 A 1002:

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.