



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:44 pm BST

PDB ID : 3AR9  
Title : Calcium pump crystal structure with bound BeF<sub>3</sub>, TNP-AMP and TG in the absence of calcium  
Authors : Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.  
Deposited on : 2010-11-24  
Resolution : 2.60 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

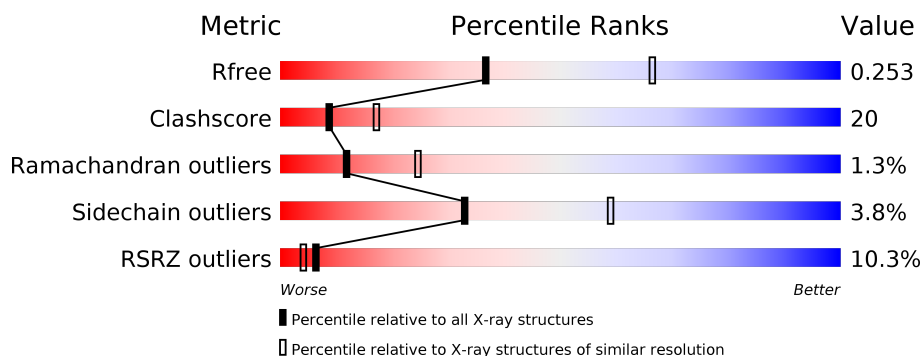
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	995	<div> <div>10%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7958 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	1	0	0
			7674	4878	1287	1452	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1A	ACE	-	ACETYLATION	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

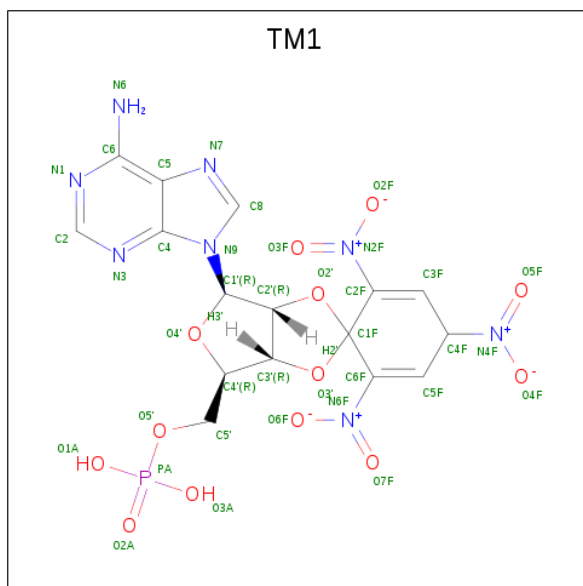
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		

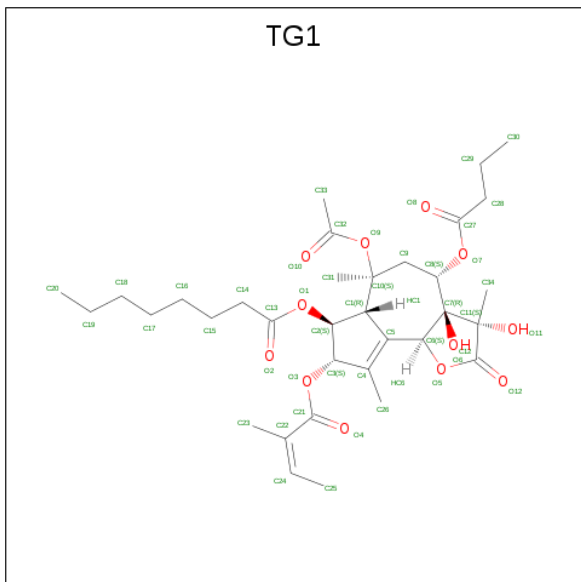
- Molecule 5 is 2',3'-O-[(1r)-2,4,6-trinitrocyclohexa-2,5-diene-1,1-diyl]adenosine 5'-(dihydrogen phosphate) (three-letter code: TM1) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>8</sub>O<sub>13</sub>P).



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

- Molecule 6 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-DECAHYD

RO-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 (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

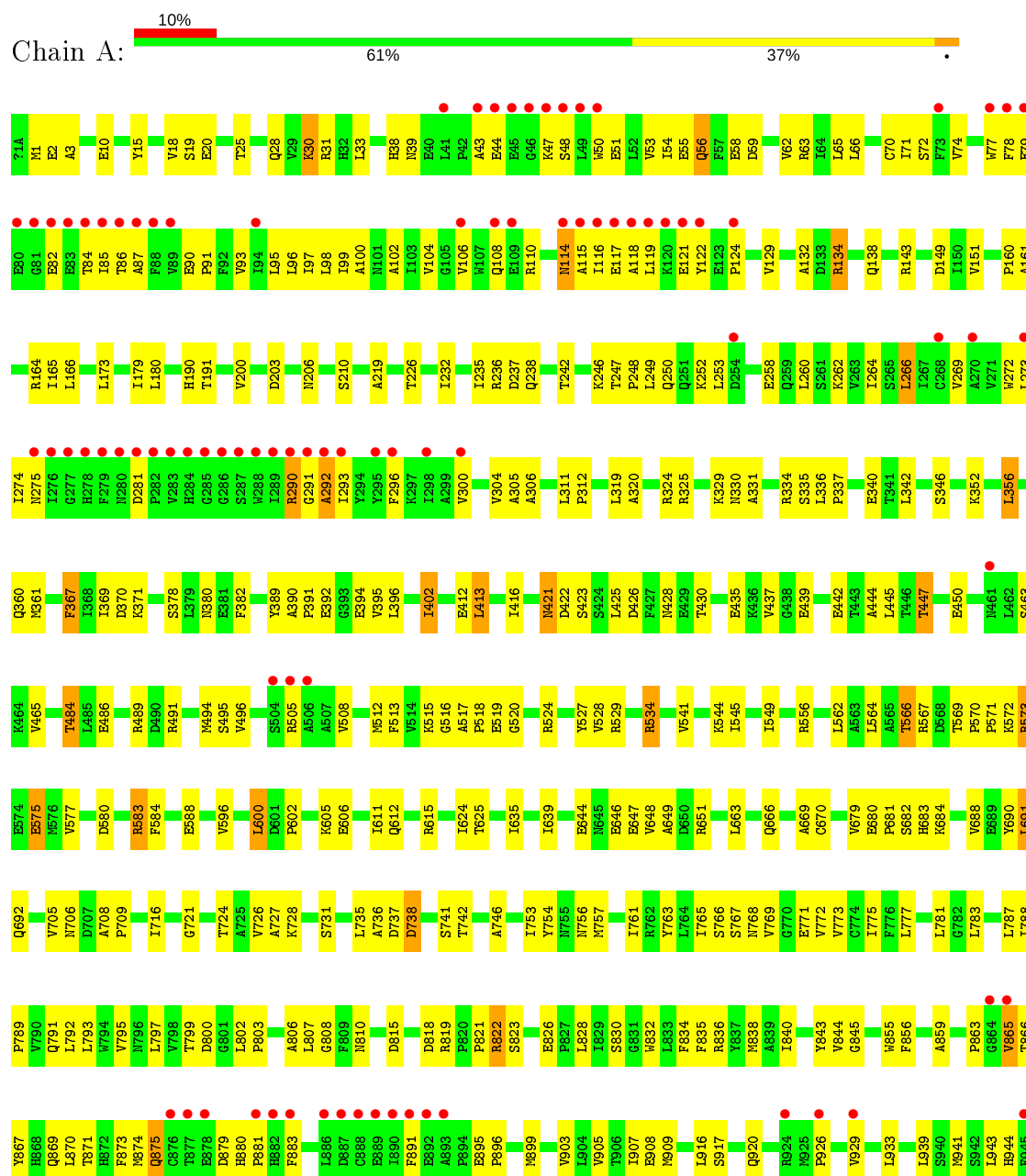
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	194	Total	O	0	0
			194	194		

### 3 Residue-property plots

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



L946	L947	L948	L949	V950	D951	P952	L953	P954	N955	I956	F957	L962	D963	L964	T965	Q966	K967	L968	N969	V970	L971	K972	I973	S974	L975	P976	V977	I978	G979	E982	I983	L984	I987	A988	R989	N990	Y991	L992	E993	G994
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.39Å 135.81Å 105.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.60 49.14 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.3 (14.97-2.60) 99.1 (49.14-2.59)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.257 0.204 , 0.253	Depositor DCC
$R_{free}$ test set	1990 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: TM1, MG, TG1, ACE, NA, BEF

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	0.36	0/7813	0.59	0/10594

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	319	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	38	0	12	1	0
6	A	46	0	50	2	0
7	A	194	0	0	5	0
All	All	7958	0	7827	319	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 20.

All (319) 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:549:ILE:HD11	1:A:596:VAL:HG21	1.48	0.96
1:A:484:THR:HB	1:A:496:VAL:HG12	1.48	0.96
1:A:573:ARG:H	1:A:573:ARG:HD2	1.36	0.91
1:A:963:ASP:HB3	1:A:966:GLN:HG3	1.51	0.90
1:A:116:ILE:HD11	1:A:236:ARG:HE	1.41	0.85
1:A:968:LEU:O	1:A:972:LYS:HG2	1.77	0.85
1:A:108:GLN:HE21	1:A:336:LEU:HD12	1.39	0.84
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.42	0.84
1:A:874:MET:HB2	1:A:875:GLN:NE2	1.94	0.82
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.60	0.81
1:A:124:PRO:HG3	1:A:160:PRO:HA	1.63	0.81
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.63	0.80
1:A:600:LEU:O	1:A:602:PRO:HD3	1.85	0.77
1:A:247:THR:HB	1:A:250:GLN:HG3	1.66	0.76
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.64	0.76
1:A:421:ASN:ND2	1:A:423:SER:H	1.85	0.75
1:A:97:ILE:HD13	1:A:797:LEU:HD11	1.69	0.75
1:A:580:ASP:O	1:A:583:ARG:HG3	1.88	0.73
1:A:606:GLU:CD	1:A:606:GLU:H	1.92	0.72
1:A:100:ALA:O	1:A:104:VAL:HG23	1.89	0.72
1:A:44:GLU:HB2	1:A:116:ILE:HD13	1.71	0.72
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.91	0.70
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.91	0.70
1:A:116:ILE:HD11	1:A:236:ARG:NE	2.07	0.70
1:A:866:THR:OG1	1:A:869:GLN:HG3	1.92	0.70
1:A:944:HIS:O	1:A:947:ILE:HG22	1.90	0.70
1:A:43:ALA:HA	1:A:116:ILE:HG21	1.74	0.69
1:A:180:LEU:O	1:A:706:ASN:HB3	1.93	0.69
1:A:899:MET:HE1	1:A:966:GLN:O	1.92	0.69
1:A:272:TRP:HA	1:A:275:ASN:HD22	1.57	0.69
1:A:757:MET:O	1:A:761:ILE:HG12	1.92	0.69
1:A:781:LEU:HB3	1:A:783:LEU:HD13	1.75	0.69
1:A:963:ASP:HB2	1:A:966:GLN:HE21	1.58	0.68
1:A:320:ALA:O	1:A:324:ARG:HG2	1.93	0.68
1:A:247:THR:HB	1:A:250:GLN:CG	2.23	0.68
1:A:108:GLN:HE21	1:A:336:LEU:CD1	2.06	0.67
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.95	0.67
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.76	0.67
1:A:238:GLN:O	1:A:242:THR:HG23	1.94	0.67
1:A:880:HIS:N	1:A:881:PRO:HD2	2.10	0.66
1:A:567:ARG:NH1	1:A:570:PRO:HA	2.11	0.66
1:A:865:VAL:HG13	1:A:869:GLN:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.77	0.66
1:A:305:ALA:HB2	1:A:792:LEU:HD13	1.78	0.66
1:A:421:ASN:HD22	1:A:422:ASP:N	1.94	0.65
1:A:247:THR:HG22	1:A:249:LEU:H	1.60	0.65
1:A:311:LEU:HD11	1:A:761:ILE:HD13	1.78	0.65
1:A:108:GLN:HG2	1:A:336:LEU:HD12	1.79	0.65
1:A:425:LEU:HD22	1:A:447:THR:HG22	1.77	0.65
1:A:979:GLY:O	1:A:983:ILE:HG12	1.98	0.64
1:A:768:ASN:O	1:A:772:VAL:HG23	1.97	0.64
1:A:486:GLU:O	1:A:491:ARG:NH2	2.30	0.64
1:A:116:ILE:HG12	1:A:236:ARG:HH21	1.63	0.64
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.79	0.64
1:A:573:ARG:H	1:A:573:ARG:CD	2.10	0.63
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.81	0.63
1:A:950:VAL:O	1:A:954:PRO:HD2	1.98	0.63
1:A:836:ARG:O	1:A:840:ILE:HG12	1.99	0.63
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.81	0.63
1:A:865:VAL:CG1	1:A:869:GLN:HB2	2.28	0.62
1:A:114:ASN:HB3	1:A:117:GLU:HB2	1.81	0.62
1:A:269:VAL:O	1:A:273:LEU:HG	2.00	0.61
1:A:249:LEU:O	1:A:253:LEU:HG	2.00	0.61
1:A:963:ASP:H	1:A:966:GLN:NE2	1.98	0.61
1:A:370:ASP:HB3	1:A:378:SER:OG	2.00	0.61
1:A:577:VAL:HB	1:A:583:ARG:NE	2.16	0.61
1:A:179:ILE:HG23	1:A:724:THR:HG21	1.83	0.61
1:A:567:ARG:NH1	1:A:571:PRO:HD3	2.16	0.61
1:A:769:VAL:HA	6:A:1003:TG1:H231	1.82	0.61
1:A:96:LEU:HD23	1:A:96:LEU:O	2.01	0.61
1:A:266:LEU:HD13	1:A:266:LEU:O	2.01	0.60
1:A:807:LEU:HA	1:A:810:ASN:OD1	2.02	0.60
1:A:767:SER:HB3	1:A:908:GLU:OE1	2.02	0.60
1:A:10:GLU:CD	1:A:10:GLU:H	2.05	0.60
1:A:258:GLU:HG2	1:A:262:LYS:NZ	2.16	0.60
1:A:300:VAL:O	1:A:304:VAL:HG23	2.03	0.59
1:A:670:CYS:HG	1:A:690:TYR:HD1	1.50	0.59
1:A:721:GLY:HA3	1:A:736:ALA:HA	1.83	0.59
1:A:84:THR:HA	1:A:87:ALA:HB2	1.83	0.59
1:A:527:TYR:HB3	1:A:534:ARG:HG3	1.83	0.59
1:A:863:PRO:HB2	1:A:865:VAL:HG23	1.83	0.59
1:A:822:ARG:HH11	1:A:826:GLU:HB3	1.68	0.59
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:O	1:A:3:ALA:HB3	2.02	0.58
1:A:421:ASN:HD22	1:A:423:SER:H	1.48	0.58
1:A:98:LEU:O	1:A:102:ALA:HB2	2.03	0.58
1:A:423:SER:HB3	1:A:437:VAL:O	2.04	0.58
1:A:856:PHE:CD1	1:A:870:LEU:HD11	2.39	0.58
1:A:161:ALA:HA	1:A:210:SER:HB2	1.85	0.58
1:A:66:LEU:HD13	1:A:98:LEU:HD13	1.85	0.58
1:A:86:THR:HG21	1:A:956:ILE:HG22	1.86	0.58
1:A:964:LEU:O	1:A:964:LEU:HD23	2.03	0.58
1:A:442:GLU:HG2	1:A:515:LYS:NZ	2.19	0.58
1:A:262:LYS:O	1:A:266:LEU:HB2	2.04	0.57
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.34	0.57
1:A:768:ASN:HB3	6:A:1003:TG1:H251	1.86	0.57
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.85	0.57
1:A:869:GLN:NE2	1:A:883:PHE:HA	2.19	0.57
1:A:726:VAL:HG23	1:A:727:ALA:N	2.19	0.57
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.31	0.57
1:A:544:LYS:O	1:A:544:LYS:HD3	2.03	0.56
1:A:290:ARG:HA	1:A:293:ILE:HG13	1.88	0.56
1:A:651:ARG:HH11	1:A:651:ARG:HG3	1.70	0.56
1:A:330:ASN:CB	1:A:737:ASP:HB2	2.36	0.56
1:A:822:ARG:HD2	1:A:823:SER:O	2.05	0.56
1:A:260:LEU:O	1:A:264:ILE:HG12	2.04	0.56
1:A:421:ASN:C	1:A:421:ASN:HD22	2.10	0.56
1:A:726:VAL:HG23	1:A:727:ALA:H	1.71	0.56
1:A:119:LEU:HD13	1:A:726:VAL:CG1	2.36	0.55
1:A:815:ASP:HA	1:A:818:ASP:OD1	2.06	0.55
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.88	0.55
1:A:330:ASN:HB2	1:A:737:ASP:HB2	1.88	0.55
1:A:494:MET:HG2	1:A:495:SER:N	2.21	0.55
1:A:232:ILE:HG13	1:A:705:VAL:HG11	1.88	0.55
1:A:771:GLU:O	1:A:775:ILE:HG12	2.07	0.55
1:A:334:ARG:CB	1:A:334:ARG:HH11	2.20	0.55
1:A:663:LEU:CD1	1:A:663:LEU:H	2.20	0.55
1:A:651:ARG:HG3	1:A:651:ARG:NH1	2.21	0.55
1:A:917:SER:OG	1:A:920:GLN:HB2	2.06	0.55
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.89	0.54
1:A:30:LYS:O	1:A:30:LYS:HD2	2.07	0.54
1:A:39:ASN:OD1	1:A:226:THR:HB	2.08	0.54
1:A:99:ILE:O	1:A:102:ALA:HB3	2.08	0.54
1:A:290:ARG:HE	1:A:290:ARG:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.90	0.53
1:A:236:ARG:HD3	1:A:236:ARG:O	2.08	0.53
1:A:20:GLU:HG3	1:A:166:LEU:HD13	1.90	0.53
1:A:463:SER:OG	1:A:465:VAL:HG23	2.09	0.53
1:A:688:VAL:O	1:A:692:GLN:HG3	2.09	0.53
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.90	0.52
1:A:567:ARG:NH1	1:A:569:THR:O	2.42	0.52
1:A:963:ASP:CB	1:A:966:GLN:HG3	2.34	0.52
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.90	0.52
1:A:335:SER:OG	1:A:337:PRO:HD2	2.09	0.52
1:A:975:LEU:N	1:A:976:PRO:HD2	2.24	0.52
1:A:840:ILE:O	1:A:844:VAL:HG23	2.10	0.52
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.92	0.52
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.92	0.52
1:A:70:CYS:O	1:A:74:VAL:HG23	2.10	0.51
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.26	0.51
1:A:963:ASP:CB	1:A:966:GLN:HE21	2.23	0.51
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.92	0.51
1:A:834:PHE:O	1:A:838:MET:HB2	2.11	0.51
1:A:62:VAL:HG13	1:A:98:LEU:HD22	1.91	0.50
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.93	0.50
1:A:72:SER:OG	1:A:91:PRO:HG3	2.11	0.50
1:A:53:VAL:O	1:A:56:GLN:HB2	2.11	0.50
1:A:670:CYS:HB3	1:A:691:LEU:CD1	2.42	0.50
1:A:238:GLN:NE2	1:A:682:SER:HB3	2.26	0.50
1:A:946:LEU:O	1:A:953:LEU:HD12	2.10	0.50
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.50
1:A:44:GLU:HB2	1:A:116:ILE:CD1	2.41	0.50
1:A:783:LEU:CD1	1:A:871:THR:HG22	2.42	0.50
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.47	0.50
1:A:969:MET:O	1:A:973:ILE:HG12	2.11	0.50
1:A:556:ARG:HG2	1:A:644:GLU:HG3	1.94	0.50
1:A:173:LEU:HD22	1:A:219:ALA:HB2	1.94	0.49
1:A:247:THR:H	1:A:250:GLN:NE2	2.10	0.49
1:A:413:LEU:HG	1:A:564:LEU:CD1	2.42	0.49
1:A:663:LEU:HD12	1:A:663:LEU:H	1.76	0.49
1:A:606:GLU:HB2	1:A:741:SER:HB3	1.94	0.49
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.93	0.49
1:A:428:ASN:OD1	1:A:430:THR:HB	2.12	0.49
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.93	0.49
1:A:108:GLN:NE2	1:A:336:LEU:HD12	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:HE22	1:A:682:SER:HB3	1.77	0.49
1:A:390:ALA:C	1:A:392:GLU:H	2.15	0.49
1:A:963:ASP:C	1:A:965:THR:H	2.14	0.49
1:A:44:GLU:CB	1:A:116:ILE:HD13	2.42	0.49
1:A:737:ASP:O	1:A:738:ASP:HB2	2.13	0.49
1:A:822:ARG:NH1	1:A:823:SER:O	2.46	0.49
1:A:905:VAL:O	1:A:909:MET:HG2	2.13	0.49
1:A:520:GLY:O	1:A:524:ARG:HG3	2.13	0.49
1:A:413:LEU:HG	1:A:564:LEU:HD12	1.93	0.49
1:A:606:GLU:CD	1:A:606:GLU:N	2.65	0.49
1:A:325:ARG:NH2	1:A:753:ILE:HD11	2.28	0.49
1:A:635:ILE:O	1:A:639:ILE:HG12	2.13	0.48
1:A:971:LEU:O	1:A:975:LEU:HD23	2.13	0.48
1:A:59:ASP:HB3	1:A:62:VAL:HG23	1.95	0.48
1:A:724:THR:O	1:A:728:LYS:HG3	2.13	0.48
1:A:77:TRP:C	1:A:79:GLU:H	2.16	0.48
1:A:93:VAL:O	1:A:97:ILE:HG13	2.13	0.48
1:A:939:LEU:O	1:A:943:LEU:HG	2.12	0.48
1:A:95:LEU:O	1:A:99:ILE:HG13	2.13	0.48
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.43	0.48
1:A:342:LEU:HD13	1:A:746:ALA:HB1	1.96	0.48
1:A:334:ARG:HD3	1:A:731:SER:O	2.14	0.48
1:A:391:PRO:HB3	1:A:450:GLU:HB3	1.96	0.48
1:A:352:LYS:HA	1:A:356:LEU:HB2	1.96	0.48
1:A:489:ARG:NH2	1:A:489:ARG:H	2.12	0.48
1:A:114:ASN:HD22	1:A:115:ALA:N	2.12	0.47
1:A:663:LEU:N	1:A:663:LEU:HD12	2.28	0.47
1:A:118:ALA:HA	1:A:121:GLU:OE2	2.13	0.47
1:A:763:TYR:O	1:A:766:SER:HB3	2.13	0.47
1:A:836:ARG:HA	1:A:984:LEU:HD13	1.97	0.47
1:A:969:MET:HE2	1:A:969:MET:O	2.14	0.47
1:A:605:LYS:HG3	7:A:2107:HOH:O	2.14	0.47
1:A:879:ASP:C	1:A:881:PRO:HD2	2.34	0.47
1:A:624:ILE:HG22	1:A:684:LYS:HG2	1.97	0.47
1:A:505:ARG:HB3	1:A:508:VAL:CG2	2.45	0.47
1:A:491:ARG:HD2	1:A:588:GLU:OE2	2.15	0.47
1:A:867:TYR:O	1:A:871:THR:HG23	2.14	0.47
1:A:873:PHE:HB2	1:A:891:PHE:CG	2.50	0.47
1:A:947:ILE:HD11	1:A:957:PHE:CD1	2.50	0.47
1:A:983:ILE:O	1:A:987:ILE:HG12	2.15	0.47
1:A:65:LEU:HB3	1:A:98:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:GLN:HA	1:A:612:GLN:NE2	2.28	0.47
1:A:761:ILE:O	1:A:765:ILE:HG12	2.13	0.47
1:A:200:VAL:HG22	1:A:203:ASP:OD2	2.15	0.47
1:A:541:VAL:O	1:A:545:ILE:HG13	2.14	0.47
1:A:342:LEU:CD1	1:A:746:ALA:HB1	2.45	0.47
1:A:875:GLN:CD	1:A:875:GLN:H	2.17	0.47
1:A:235:ILE:HD11	1:A:681:PRO:HG2	1.96	0.46
1:A:795:VAL:HG13	1:A:799:THR:HB	1.97	0.46
1:A:71:ILE:HG21	1:A:296:PHE:HB3	1.98	0.46
1:A:600:LEU:HD13	1:A:600:LEU:O	2.16	0.46
1:A:963:ASP:C	1:A:965:THR:N	2.69	0.46
1:A:235:ILE:CD1	1:A:681:PRO:HG2	2.46	0.46
1:A:334:ARG:HB3	1:A:334:ARG:NH1	2.30	0.46
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.97	0.46
1:A:947:ILE:HD11	1:A:957:PHE:CD2	2.50	0.46
1:A:311:LEU:HD11	1:A:761:ILE:CD1	2.45	0.46
1:A:122:TYR:CZ	1:A:179:ILE:HG21	2.50	0.46
1:A:247:THR:HG22	1:A:249:LEU:N	2.29	0.46
1:A:756:ASN:OD1	1:A:810:ASN:HB2	2.15	0.46
1:A:367:PHE:C	1:A:367:PHE:CD2	2.89	0.46
1:A:442:GLU:HG2	1:A:515:LYS:HZ2	1.81	0.46
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.98	0.46
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.96	0.46
1:A:346:SER:HA	1:A:821:PRO:HG2	1.97	0.45
1:A:50:TRP:O	1:A:54:ILE:HG12	2.16	0.45
1:A:402:ILE:HB	7:A:2221:HOH:O	2.15	0.45
1:A:737:ASP:HB3	7:A:2062:HOH:O	2.16	0.45
1:A:25:THR:HA	1:A:132:ALA:HB3	1.98	0.45
1:A:272:TRP:HA	1:A:275:ASN:ND2	2.28	0.45
1:A:134:ARG:HG2	1:A:138:GLN:OE1	2.15	0.45
1:A:584:PHE:N	1:A:584:PHE:CD2	2.84	0.45
1:A:44:GLU:OE1	1:A:115:ALA:HB3	2.17	0.45
1:A:425:LEU:HD12	1:A:435:GLU:O	2.16	0.45
1:A:235:ILE:HG21	1:A:705:VAL:HG12	1.98	0.45
1:A:389:TYR:HA	1:A:447:THR:HG21	1.98	0.45
1:A:249:LEU:HD13	1:A:754:TYR:HE1	1.81	0.45
1:A:806:ALA:HB1	1:A:933:LEU:HA	1.98	0.45
1:A:516:GLY:HA2	5:A:1002:TM1:O6F	2.17	0.44
1:A:86:THR:CG2	1:A:956:ILE:HG22	2.47	0.44
1:A:246:LYS:HB3	1:A:250:GLN:HE21	1.82	0.44
1:A:38:HIS:CD2	1:A:143:ARG:NH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG12	1:A:402:ILE:CD1	2.46	0.44
1:A:666:GLN:O	1:A:669:ALA:HB3	2.18	0.44
1:A:615:ARG:HG2	7:A:2103:HOH:O	2.16	0.44
1:A:102:ALA:O	1:A:106:VAL:HG23	2.18	0.44
1:A:978:ILE:O	1:A:982:GLU:HB2	2.18	0.43
1:A:161:ALA:CA	1:A:210:SER:HB2	2.49	0.43
1:A:329:LYS:O	1:A:330:ASN:HB2	2.19	0.43
1:A:646:GLU:HG2	1:A:647:GLU:N	2.32	0.43
1:A:941:MET:O	1:A:944:HIS:HB3	2.19	0.43
1:A:735:LEU:C	1:A:737:ASP:H	2.22	0.43
1:A:787:LEU:HA	1:A:791:GLN:OE1	2.19	0.43
1:A:38:HIS:CD2	1:A:143:ARG:CZ	3.01	0.43
1:A:236:ARG:HD3	1:A:236:ARG:C	2.38	0.43
1:A:416:ILE:HG23	1:A:513:PHE:HB3	2.00	0.43
1:A:735:LEU:C	1:A:737:ASP:N	2.71	0.43
1:A:90:GLU:CB	1:A:91:PRO:HD3	2.45	0.43
1:A:993:GLU:OE1	1:A:993:GLU:HA	2.18	0.43
1:A:625:THR:O	1:A:679:VAL:HG22	2.19	0.43
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.83	0.43
1:A:947:ILE:HA	1:A:953:LEU:CD1	2.49	0.43
1:A:247:THR:HG23	1:A:248:PRO:HD2	2.01	0.43
1:A:59:ASP:HB3	1:A:62:VAL:CG2	2.49	0.43
1:A:838:MET:CE	1:A:838:MET:HA	2.49	0.43
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.49	0.43
1:A:974:SER:C	1:A:976:PRO:HD2	2.40	0.43
1:A:815:ASP:CG	1:A:819:ARG:HH21	2.23	0.42
1:A:572:LYS:HB2	1:A:575:GLU:HG2	2.00	0.42
1:A:663:LEU:CD1	1:A:663:LEU:N	2.83	0.42
1:A:777:LEU:O	1:A:781:LEU:HD13	2.18	0.42
1:A:830:SER:HA	1:A:834:PHE:HB2	2.01	0.42
1:A:810:ASN:HD21	1:A:916:LEU:HA	1.85	0.42
1:A:880:HIS:N	1:A:881:PRO:CD	2.80	0.42
1:A:190:HIS:O	1:A:206:ASN:HA	2.19	0.42
1:A:247:THR:HB	1:A:250:GLN:CD	2.39	0.42
1:A:926:PRO:O	1:A:929:VAL:HG23	2.19	0.42
1:A:836:ARG:HG2	1:A:984:LEU:HD13	2.01	0.42
1:A:1:MET:HB2	1:A:15:TYR:CE1	2.55	0.42
1:A:380:ASN:HB3	1:A:382:PHE:CE1	2.55	0.42
1:A:304:VAL:HG13	1:A:793:LEU:HD21	2.02	0.42
1:A:781:LEU:CB	1:A:783:LEU:HD13	2.47	0.42
1:A:799:THR:HG21	1:A:905:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLU:O	1:A:683:HIS:HB2	2.20	0.41
1:A:85:ILE:HG23	1:A:86:THR:HG23	2.02	0.41
1:A:952:PRO:O	1:A:956:ILE:HG12	2.20	0.41
1:A:975:LEU:CD2	1:A:975:LEU:H	2.33	0.41
1:A:611:ILE:O	1:A:615:ARG:HG3	2.21	0.41
1:A:789:PRO:O	1:A:793:LEU:HG	2.21	0.41
1:A:58:GLU:O	1:A:63:ARG:NH2	2.52	0.41
1:A:990:ASN:C	1:A:992:LEU:H	2.22	0.41
1:A:18:VAL:HG22	1:A:19:SER:N	2.35	0.41
1:A:600:LEU:C	1:A:600:LEU:HD13	2.41	0.41
1:A:252:LYS:HG2	1:A:828:LEU:HD13	2.03	0.41
1:A:28:GLN:HG2	1:A:31:ARG:HH22	1.85	0.41
1:A:48:SER:OG	1:A:51:GLU:HG2	2.20	0.41
1:A:788:ILE:HG13	1:A:791:GLN:HG3	2.03	0.41
1:A:800:ASP:O	1:A:803:PRO:HD2	2.21	0.41
1:A:873:PHE:HB2	1:A:891:PHE:CD1	2.56	0.41
1:A:903:VAL:O	1:A:907:ILE:HG13	2.21	0.41
1:A:237:ASP:O	1:A:238:GLN:C	2.59	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.84	0.41
1:A:97:ILE:CD1	1:A:797:LEU:HD11	2.44	0.41
1:A:371:LYS:HB2	7:A:2296:HOH:O	2.22	0.40
1:A:165:ILE:HG22	1:A:191:THR:HG22	2.03	0.40
1:A:962:LEU:HB3	1:A:966:GLN:HB2	2.02	0.40
1:A:291:GLY:O	1:A:292:ALA:HB2	2.21	0.40
1:A:360:GLN:O	1:A:361:MET:C	2.60	0.40
1:A:389:TYR:HB3	1:A:425:LEU:CD1	2.51	0.40
1:A:51:GLU:O	1:A:55:GLU:HG2	2.21	0.40
1:A:71:ILE:CG2	1:A:296:PHE:HB3	2.51	0.40
1:A:815:ASP:OD1	1:A:819:ARG:NH2	2.54	0.40
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.94	0.40
1:A:832:TRP:O	1:A:835:PHE:HB3	2.22	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	993/995 (100%)	910 (92%)	70 (7%)	13 (1%)	12	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ALA
1	A	649	ALA
1	A	47	LYS
1	A	78	PHE
1	A	82	GLU
1	A	991	TYR
1	A	575	GLU
1	A	519	GLU
1	A	875	GLN
1	A	951	ASP
1	A	865	VAL
1	A	274	ILE
1	A	648	VAL

### 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%)	808 (96%)	32 (4%)	33	59

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	33	LEU
1	A	56	GLN
1	A	114	ASN
1	A	134	ARG
1	A	149	ASP

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	266	LEU
1	A	281	ASP
1	A	290	ARG
1	A	319	LEU
1	A	340	GLU
1	A	356	LEU
1	A	367	PHE
1	A	402	ILE
1	A	413	LEU
1	A	421	ASN
1	A	426	ASP
1	A	439	GLU
1	A	445	LEU
1	A	447	THR
1	A	484	THR
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	573	ARG
1	A	583	ARG
1	A	600	LEU
1	A	691	LEU
1	A	738	ASP
1	A	822	ARG
1	A	955	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	101	ASN
1	A	108	GLN
1	A	114	ASN
1	A	177	GLN
1	A	238	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	406	GLN
1	A	421	ASN
1	A	456	ASN

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Mol	Chain	Res	Type
1	A	510	ASN
1	A	612	GLN
1	A	875	GLN
1	A	911	ASN
1	A	914	ASN
1	A	966	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	TM1	A	1002	-	30,42,42	3.54	12 (40%)	31,66,66	3.02	11 (35%)
6	TG1	A	1003	-	43,48,48	1.77	10 (23%)	44,72,72	1.85	10 (22%)
4	BEF	A	998	1	0,3,3	0.00	-	-		

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	TM1	A	1002	-	-	4/12/68/68	0/5/5/5
6	TG1	A	1003	-	-	15/33/99/99	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	TM1	C5F-C6F	12.27	1.51	1.33
5	A	1002	TM1	O3'-C1F	7.05	1.51	1.41
6	A	1003	TG1	O4-C21	6.99	1.36	1.21
5	A	1002	TM1	O2'-C1F	6.49	1.50	1.41
5	A	1002	TM1	C3F-C2F	4.17	1.39	1.33
5	A	1002	TM1	C4F-C3F	-3.95	1.38	1.50
5	A	1002	TM1	C4-N3	3.92	1.41	1.35
5	A	1002	TM1	C2-N3	3.84	1.38	1.32
5	A	1002	TM1	C5'-C4'	3.55	1.62	1.51
6	A	1003	TG1	C9-C10	3.32	1.59	1.54
6	A	1003	TG1	C3-C4	3.16	1.54	1.50
5	A	1002	TM1	C3'-C4'	-3.11	1.44	1.52
5	A	1002	TM1	C2-N1	3.07	1.39	1.33
5	A	1002	TM1	O7F-N6F	-3.04	1.17	1.22
5	A	1002	TM1	C4F-C5F	-2.49	1.42	1.50
6	A	1003	TG1	C1-C2	2.47	1.58	1.54
6	A	1003	TG1	O6-C7	2.29	1.47	1.43
6	A	1003	TG1	C34-C11	2.25	1.56	1.53
6	A	1003	TG1	C1-C5	2.17	1.54	1.51
6	A	1003	TG1	C9-C8	2.15	1.55	1.52
6	A	1003	TG1	C11-C7	2.10	1.58	1.55
6	A	1003	TG1	C31-C10	2.08	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	TM1	O2'-C1F-C2F	-8.58	98.73	110.47
6	A	1003	TG1	C10-O9-C32	7.21	138.64	121.53
5	A	1002	TM1	O3'-C1F-C6F	-7.06	100.81	110.47
5	A	1002	TM1	O2'-C2'-C3'	6.84	114.50	103.58
5	A	1002	TM1	N3-C2-N1	-4.74	121.27	128.68
5	A	1002	TM1	O4'-C1'-C2'	-4.47	98.83	106.59
5	A	1002	TM1	O3'-C1F-C2F	3.96	115.89	110.47
5	A	1002	TM1	C2'-C3'-C4'	3.60	112.28	103.72
6	A	1003	TG1	O12-C12-C11	-3.36	124.90	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1003	TG1	O3-C21-O4	3.16	129.34	123.32
6	A	1003	TG1	C7-C6-C5	3.01	123.11	115.41
6	A	1003	TG1	C24-C22-C21	2.84	132.01	120.78
6	A	1003	TG1	C11-C7-C6	-2.74	97.74	103.03
6	A	1003	TG1	O5-C12-O12	2.55	125.00	121.62
5	A	1002	TM1	O5'-C5'-C4'	2.53	117.69	108.99
5	A	1002	TM1	O3'-C3'-C2'	2.44	107.48	103.58
6	A	1003	TG1	C23-C22-C21	-2.38	110.14	116.09
6	A	1003	TG1	O7-C8-C9	2.31	110.76	106.63
5	A	1002	TM1	O2'-C2'-C1'	2.24	116.18	109.75
6	A	1003	TG1	O11-C11-C12	-2.13	99.12	106.32
5	A	1002	TM1	O4'-C4'-C3'	-2.05	100.48	104.87

There are no chirality outliers.

All (19) torsion outliers are listed below:

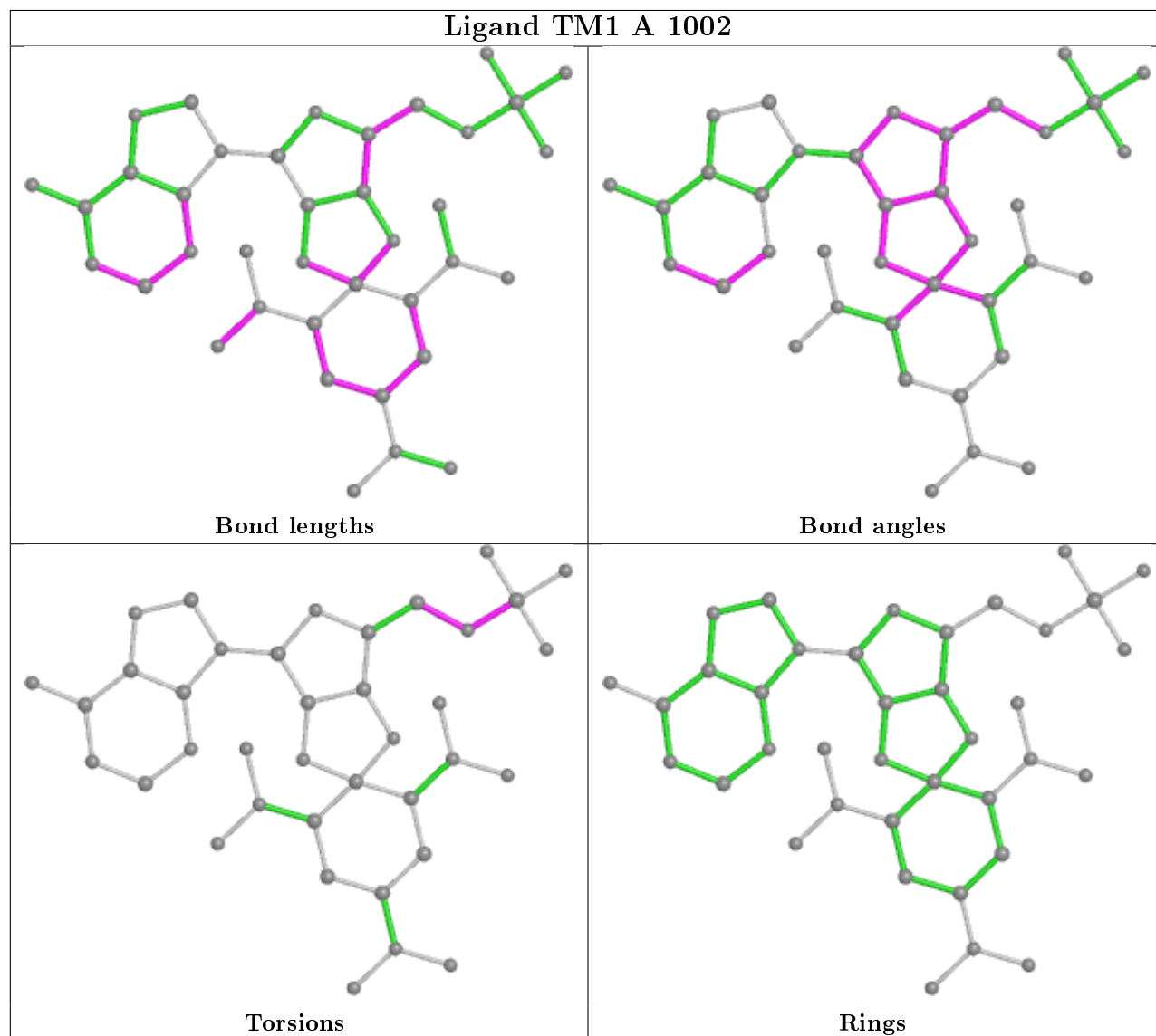
Mol	Chain	Res	Type	Atoms
5	A	1002	TM1	C5'-O5'-PA-O1A
5	A	1002	TM1	C5'-O5'-PA-O2A
5	A	1002	TM1	C5'-O5'-PA-O3A
6	A	1003	TG1	C9-C10-O9-C32
6	A	1003	TG1	C1-C10-O9-C32
6	A	1003	TG1	C31-C10-O9-C32
6	A	1003	TG1	O3-C21-C22-C23
6	A	1003	TG1	O3-C21-C22-C24
6	A	1003	TG1	O4-C21-C22-C23
6	A	1003	TG1	O4-C21-C22-C24
6	A	1003	TG1	C14-C15-C16-C17
6	A	1003	TG1	C15-C16-C17-C18
6	A	1003	TG1	C17-C18-C19-C20
6	A	1003	TG1	C22-C21-O3-C3
5	A	1002	TM1	C4'-C5'-O5'-PA
6	A	1003	TG1	O1-C13-C14-C15
6	A	1003	TG1	O7-C27-C28-C29
6	A	1003	TG1	O8-C27-C28-C29
6	A	1003	TG1	O2-C13-C14-C15

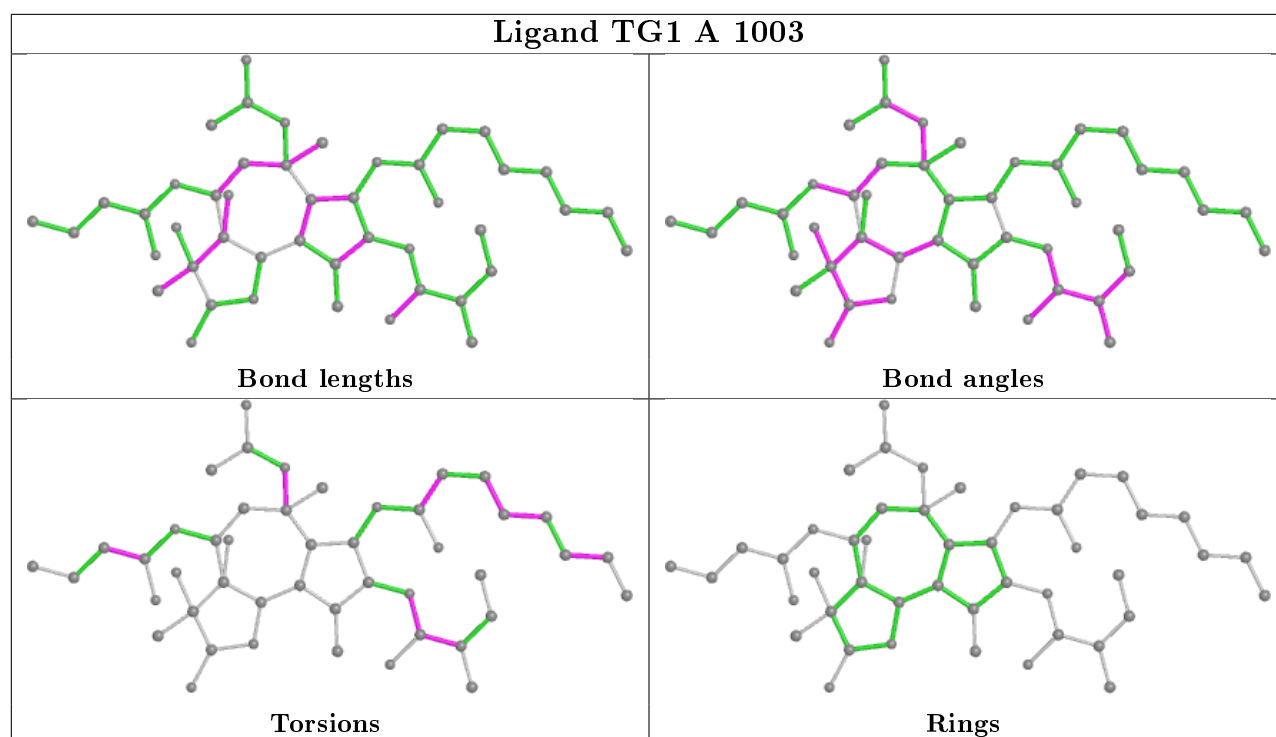
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	TM1	1	0
6	A	1003	TG1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	994/995 (99%)	0.44	102 (10%) 6 4	33, 64, 135, 178	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ASN	15.0
1	A	284	HIS	11.8
1	A	886	LEU	10.9
1	A	116	ILE	8.0
1	A	994	GLY	7.9
1	A	120	LYS	7.4
1	A	891	PHE	7.2
1	A	286	GLY	7.2
1	A	124	PRO	7.1
1	A	45	GLU	7.1
1	A	276	ILE	7.0
1	A	117	GLU	7.0
1	A	289	ILE	7.0
1	A	282	PRO	6.9
1	A	115	ALA	6.9
1	A	883	PHE	6.7
1	A	279	PHE	6.7
1	A	83	GLU	6.6
1	A	889	GLU	6.5
1	A	49	LEU	6.5
1	A	993	GLU	6.5
1	A	285	GLY	6.3
1	A	43	ALA	6.2
1	A	119	LEU	6.1
1	A	85	ILE	6.0
1	A	80	GLU	5.8
1	A	114	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLY	5.3
1	A	82	GLU	5.1
1	A	81	GLY	5.1
1	A	78	PHE	4.8
1	A	278	HIS	4.6
1	A	876	CYS	4.5
1	A	79	GLU	4.4
1	A	281	ASP	4.4
1	A	955	MET	4.3
1	A	877	THR	4.2
1	A	461	ASN	4.2
1	A	121	GLU	4.1
1	A	950	VAL	4.0
1	A	292	ALA	4.0
1	A	945	PHE	4.0
1	A	283	VAL	4.0
1	A	882	HIS	3.8
1	A	254	ASP	3.8
1	A	949	TYR	3.7
1	A	293	ILE	3.7
1	A	946	LEU	3.6
1	A	288	TRP	3.6
1	A	506	ALA	3.5
1	A	273	LEU	3.5
1	A	44	GLU	3.5
1	A	948	LEU	3.4
1	A	270	ALA	3.4
1	A	887	ASP	3.4
1	A	878	GLU	3.4
1	A	84	THR	3.3
1	A	122	TYR	3.3
1	A	924	ARG	3.3
1	A	881	PRO	3.3
1	A	295	TYR	3.2
1	A	890	ILE	3.2
1	A	975	LEU	3.2
1	A	89	VAL	3.2
1	A	77	TRP	3.1
1	A	951	ASP	3.1
1	A	108	GLN	3.1
1	A	46	GLY	3.0
1	A	47	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	926	PRO	2.9
1	A	50	TRP	2.8
1	A	87	ALA	2.8
1	A	888	CYS	2.8
1	A	291	GLY	2.8
1	A	287	SER	2.8
1	A	88	PHE	2.7
1	A	118	ALA	2.7
1	A	505	ARG	2.7
1	A	86	THR	2.5
1	A	296	PHE	2.5
1	A	953	LEU	2.4
1	A	929	VAL	2.4
1	A	300	VAL	2.4
1	A	988	ALA	2.4
1	A	275	ASN	2.3
1	A	106	VAL	2.3
1	A	864	GLY	2.3
1	A	964	LEU	2.3
1	A	893	ALA	2.3
1	A	268	CYS	2.2
1	A	892	GLU	2.2
1	A	48	SER	2.2
1	A	952	PRO	2.2
1	A	109	GLU	2.2
1	A	298	ILE	2.2
1	A	73	PHE	2.2
1	A	290	ARG	2.2
1	A	957	PHE	2.2
1	A	41	LEU	2.1
1	A	94	ILE	2.1
1	A	865	VAL	2.0
1	A	504	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

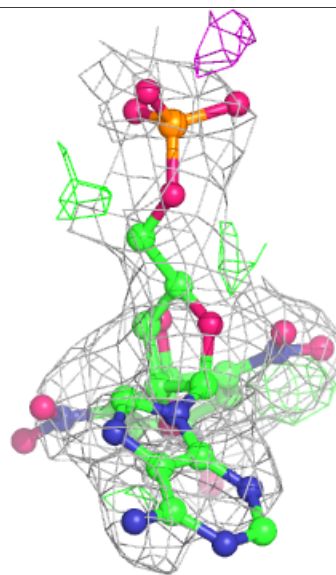
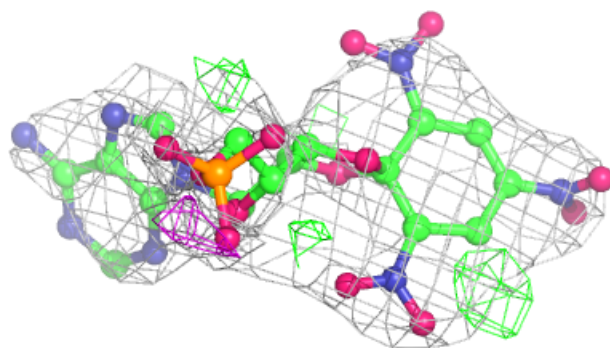
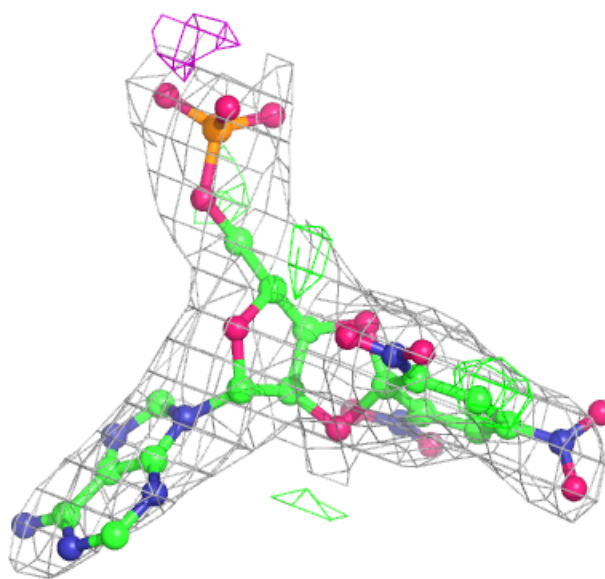
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

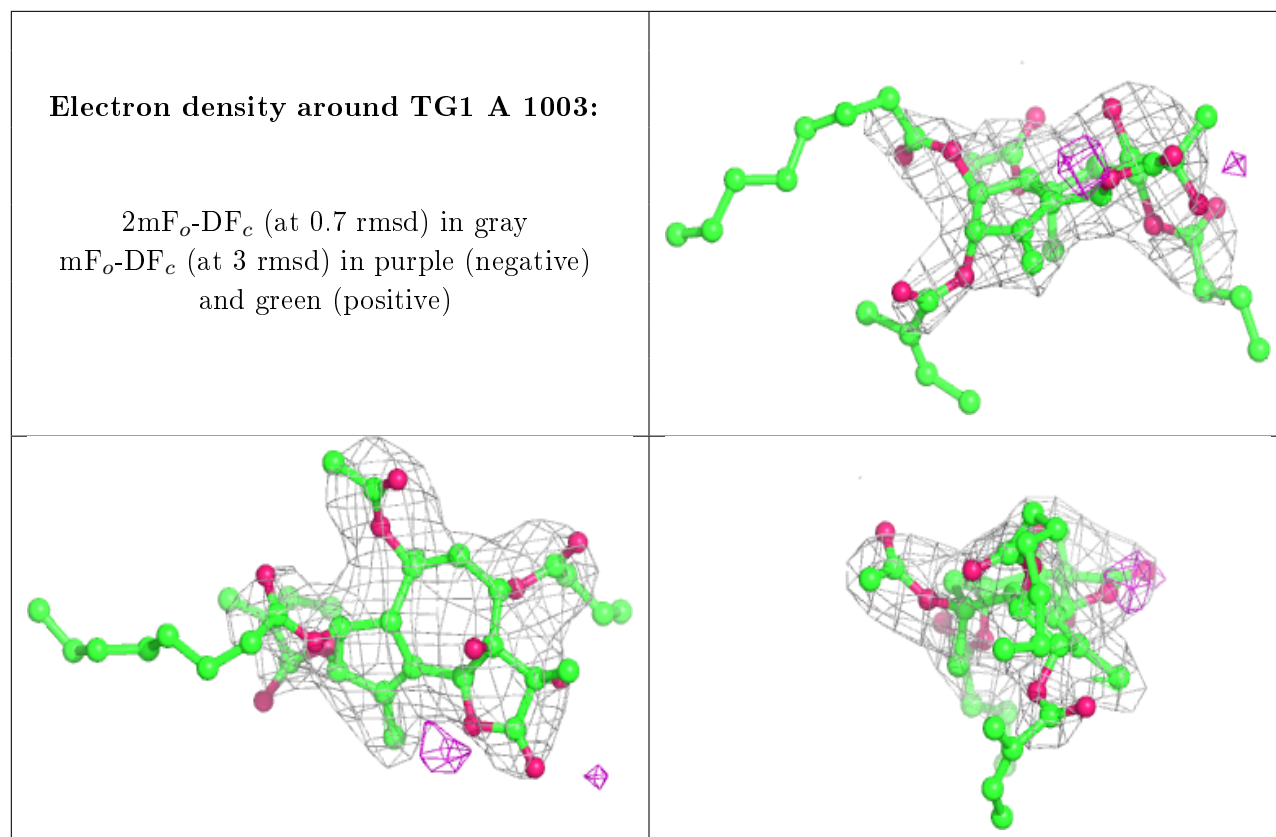
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TM1	A	1002	38/38	0.84	0.25	106,112,115,117	0
6	TG1	A	1003	46/46	0.91	0.35	92,97,109,110	0
2	NA	A	1000	1/1	0.92	0.07	54,54,54,54	0
3	MG	A	997	1/1	0.99	0.16	38,38,38,38	0
4	BEF	A	998	4/4	0.99	0.13	41,42,43,43	0

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 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.