



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:40 am BST

PDB ID : 2ZBG  
Title : Calcium pump crystal structure with bound AlF<sub>4</sub> and TG in the absence of calcium  
Authors : Toyoshima, C.; Ogawa, H.; Norimatsu, Y.  
Deposited on : 2007-10-20  
Resolution : 2.55 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 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

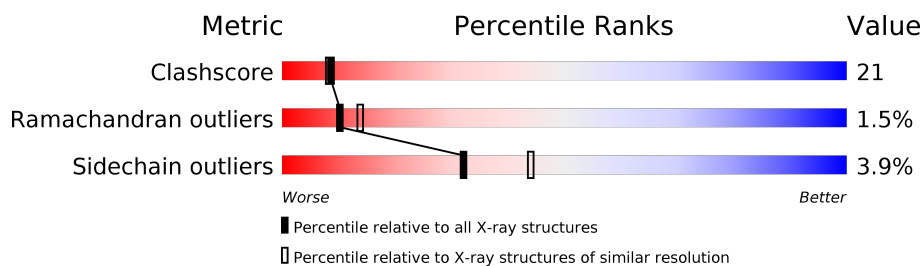
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7884 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			

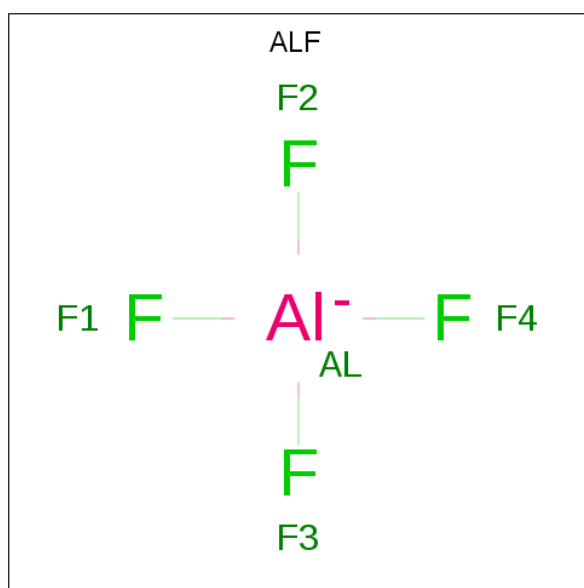
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

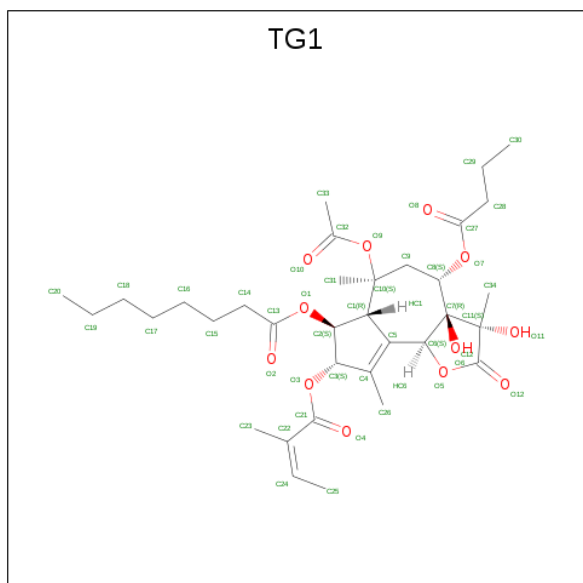
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BAPHA]]-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 (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

- Molecule 5 is water.

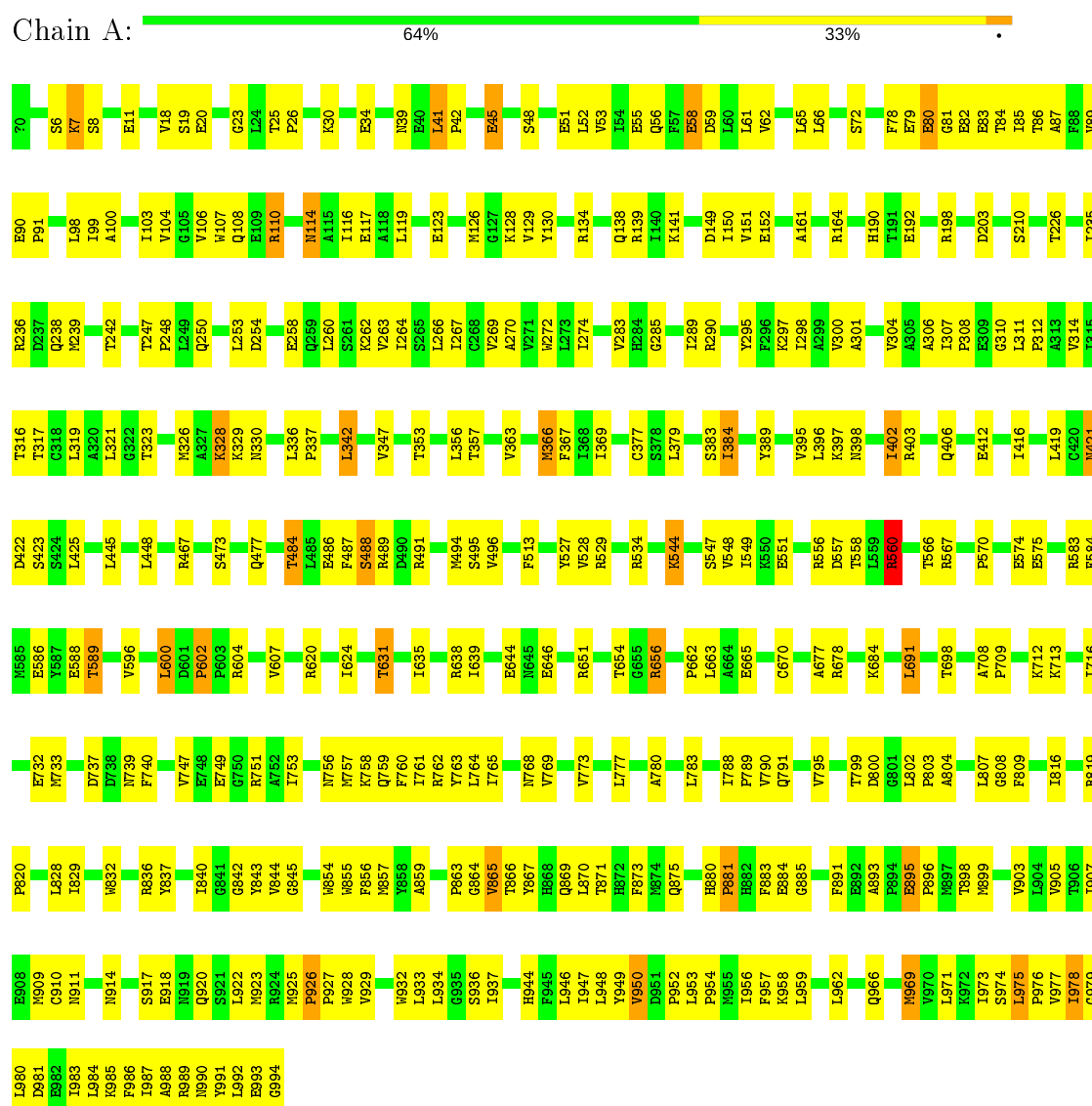
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		

### 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.50 Å   70.20 Å   143.40 Å 90.00°   106.80°   90.00°	Depositor
Resolution (Å)	11.99 – 2.55	Depositor
% Data completeness (in resolution range)	98.6 (11.99-2.55)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, TG1, ACE

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	0.49	0/7813	0.67	6/10594 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	290	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	A	110	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	560	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	A	969	MET	CG-SD-CE	6.09	109.95	100.20
1	A	366	MET	CG-SD-CE	5.94	109.70	100.20
1	A	556	ARG	NE-CZ-NH2	5.35	122.97	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ALA	Mainchain
1	A	602	PRO	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7674	0	7765	320	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	46	0	50	2	0
5	A	158	0	0	2	0
All	All	7884	0	7815	320	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 21.

All (320) 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:55:GLU:HA	1:A:58:GLU:CD	1.86	0.95
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.48	0.94
1:A:421:ASN:ND2	1:A:423:SER:H	1.64	0.94
1:A:557:ASP:HA	1:A:638:ARG:HH22	1.31	0.93
1:A:53:VAL:O	1:A:56:GLN:HB2	1.73	0.88
1:A:557:ASP:HA	1:A:638:ARG:NH2	1.89	0.86
1:A:762:ARG:HG2	1:A:829:ILE:HD11	1.54	0.86
1:A:631:THR:HG21	5:A:2081:HOH:O	1.78	0.84
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.80	0.82
1:A:421:ASN:HD22	1:A:422:ASP:N	1.75	0.82
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.63	0.80
1:A:971:LEU:O	1:A:975:LEU:HB2	1.82	0.79
1:A:840:ILE:HD13	1:A:980:LEU:HD23	1.64	0.78
1:A:917:SER:OG	1:A:920:GLN:HB2	1.83	0.78
1:A:55:GLU:HA	1:A:58:GLU:CG	2.13	0.78
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.66	0.77
1:A:557:ASP:CA	1:A:638:ARG:HH22	1.96	0.77
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.65	0.77
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.67	0.76
1:A:20:GLU:HA	1:A:150:ILE:CD1	2.16	0.76
1:A:274:ILE:HG21	1:A:780:ALA:HB1	1.66	0.76
1:A:242:THR:HG21	1:A:712:LYS:HG2	1.65	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:HD13	1:A:600:LEU:O	1.86	0.75
1:A:866:THR:OG1	1:A:869:GLN:HG2	1.87	0.75
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.70	0.73
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.70	0.73
1:A:119:LEU:HD22	1:A:239:MET:HE3	1.70	0.72
1:A:289:ILE:H	1:A:289:ILE:HD12	1.51	0.72
1:A:55:GLU:HA	1:A:58:GLU:HG3	1.71	0.72
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.71	0.72
1:A:895:GLU:H	1:A:896:PRO:HD2	1.53	0.71
1:A:301:ALA:HA	1:A:789:PRO:HB3	1.72	0.70
1:A:81:GLY:HA2	1:A:84:THR:HB	1.72	0.70
1:A:41:LEU:HB2	1:A:123:GLU:OE1	1.92	0.70
1:A:119:LEU:HD22	1:A:239:MET:CE	2.22	0.69
1:A:646:GLU:OE2	1:A:651:ARG:NH1	2.24	0.69
1:A:82:GLU:HG3	1:A:83:GLU:HG3	1.75	0.68
1:A:865:VAL:CG1	1:A:869:GLN:HG3	2.23	0.68
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.75	0.68
1:A:311:LEU:HD11	1:A:761:ILE:HD13	1.76	0.67
1:A:788:ILE:HD13	1:A:958:LYS:HE2	1.75	0.67
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.75	0.67
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.25	0.67
1:A:567:ARG:CD	1:A:570:PRO:HA	2.25	0.67
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.77	0.67
1:A:800:ASP:O	1:A:803:PRO:HD2	1.95	0.66
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.78	0.66
1:A:48:SER:OG	1:A:51:GLU:HG2	1.97	0.65
1:A:23:GLY:HA3	1:A:130:TYR:O	1.97	0.64
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.79	0.64
1:A:769:VAL:HA	4:A:1003:TG1:H231	1.78	0.64
1:A:662:PRO:HD2	1:A:665:GLU:HG3	1.79	0.64
1:A:865:VAL:HG13	1:A:869:GLN:HG3	1.78	0.64
1:A:910:CYS:HB3	1:A:978:ILE:HD11	1.80	0.64
1:A:247:THR:OG1	1:A:248:PRO:HD2	1.98	0.64
1:A:55:GLU:HA	1:A:58:GLU:OE1	1.98	0.63
1:A:484:THR:HB	1:A:496:VAL:HG12	1.81	0.63
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.81	0.63
1:A:749:GLU:O	1:A:753:ILE:HG12	1.98	0.63
1:A:791:GLN:NE2	1:A:959:LEU:HD21	2.14	0.63
1:A:869:GLN:HB2	1:A:883:PHE:CD1	2.34	0.63
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.80	0.63
1:A:283:VAL:HG22	1:A:285:GLY:H	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:LEU:O	1:A:953:LEU:HD12	1.99	0.62
1:A:926:PRO:O	1:A:929:VAL:HG23	1.99	0.62
1:A:45:GLU:H	1:A:45:GLU:CD	2.02	0.62
1:A:975:LEU:N	1:A:976:PRO:HD2	2.15	0.61
1:A:247:THR:HG22	1:A:250:GLN:CG	2.31	0.61
1:A:974:SER:C	1:A:976:PRO:HD2	2.21	0.60
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.83	0.60
1:A:977:VAL:C	1:A:979:GLY:H	2.03	0.60
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.84	0.60
1:A:308:PRO:HA	1:A:768:ASN:HD21	1.66	0.60
1:A:600:LEU:O	1:A:602:PRO:HD3	2.02	0.60
1:A:30:LYS:O	1:A:34:GLU:HG3	2.02	0.60
1:A:832:TRP:CD1	1:A:988:ALA:HB2	2.37	0.60
1:A:873:PHE:HB2	1:A:891:PHE:CE1	2.37	0.60
1:A:53:VAL:O	1:A:56:GLN:CB	2.47	0.59
1:A:836:ARG:HG3	1:A:984:LEU:HD13	1.83	0.59
1:A:55:GLU:CA	1:A:58:GLU:OE1	2.51	0.59
1:A:326:MET:CG	1:A:749:GLU:HG2	2.33	0.59
1:A:89:VAL:HG11	1:A:956:ILE:HB	1.84	0.58
1:A:395:VAL:O	1:A:402:ILE:HD13	2.03	0.58
1:A:59:ASP:OD2	1:A:62:VAL:HG23	2.02	0.58
1:A:289:ILE:N	1:A:289:ILE:HD12	2.17	0.58
1:A:764:LEU:HD11	1:A:804:ALA:HB2	1.83	0.58
1:A:25:THR:HB	1:A:26:PRO:HD2	1.85	0.58
1:A:905:VAL:O	1:A:909:MET:HG2	2.04	0.58
1:A:247:THR:CG2	1:A:250:GLN:H	2.16	0.57
1:A:116:ILE:H	1:A:116:ILE:HD12	1.69	0.57
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.87	0.57
1:A:7:LYS:N	1:A:7:LYS:HD2	2.19	0.57
1:A:247:THR:HG22	1:A:250:GLN:HG3	1.86	0.57
1:A:104:VAL:O	1:A:107:TRP:HB3	2.05	0.57
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.40	0.57
1:A:41:LEU:HG	1:A:236:ARG:HG3	1.87	0.57
1:A:55:GLU:CA	1:A:58:GLU:HG3	2.34	0.57
1:A:866:THR:HG23	1:A:869:GLN:NE2	2.19	0.57
1:A:89:VAL:HG21	1:A:956:ILE:HG22	1.86	0.56
1:A:917:SER:HB2	1:A:925:MET:SD	2.45	0.56
1:A:948:LEU:O	1:A:954:PRO:HG3	2.06	0.56
1:A:950:VAL:O	1:A:954:PRO:HD2	2.04	0.56
1:A:297:LYS:O	1:A:300:VAL:HG22	2.05	0.56
1:A:757:MET:O	1:A:761:ILE:HG12	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:HIS:O	1:A:884:GLU:HB2	2.05	0.56
1:A:866:THR:HG23	1:A:869:GLN:HE21	1.72	0.56
1:A:289:ILE:H	1:A:289:ILE:CD1	2.19	0.55
1:A:310:GLY:O	1:A:314:VAL:HG23	2.07	0.55
1:A:6:SER:C	1:A:7:LYS:HD2	2.26	0.55
1:A:99:ILE:O	1:A:103:ILE:HG13	2.07	0.55
1:A:863:PRO:C	1:A:865:VAL:H	2.10	0.54
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.88	0.54
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.88	0.54
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.07	0.54
1:A:473:SER:O	1:A:477:GLN:HG2	2.07	0.54
1:A:893:ALA:O	1:A:896:PRO:HD2	2.08	0.54
1:A:403:ARG:HB2	1:A:406:GLN:HG2	1.89	0.54
1:A:421:ASN:HD22	1:A:423:SER:H	1.49	0.54
1:A:758:LYS:HE3	1:A:762:ARG:NH2	2.24	0.53
1:A:116:ILE:N	1:A:116:ILE:HD12	2.24	0.53
1:A:954:PRO:HB2	1:A:959:LEU:O	2.07	0.53
1:A:342:LEU:HG	1:A:716:ILE:HG21	1.90	0.53
1:A:421:ASN:C	1:A:421:ASN:HD22	2.12	0.53
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.91	0.53
1:A:800:ASP:C	1:A:803:PRO:HD2	2.28	0.53
1:A:600:LEU:HD13	1:A:600:LEU:C	2.30	0.53
1:A:66:LEU:HD13	1:A:98:LEU:HD13	1.90	0.53
1:A:269:VAL:O	1:A:272:TRP:HB3	2.09	0.53
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.89	0.52
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.91	0.52
1:A:383:SER:OG	1:A:396:LEU:HB2	2.09	0.52
1:A:421:ASN:HD22	1:A:422:ASP:H	1.57	0.52
1:A:295:TYR:HA	1:A:298:ILE:HG12	1.92	0.52
1:A:297:LYS:O	1:A:300:VAL:CG2	2.58	0.52
1:A:898:THR:O	1:A:962:LEU:HD11	2.09	0.52
1:A:944:HIS:O	1:A:947:ILE:HG22	2.10	0.52
1:A:950:VAL:CG1	1:A:952:PRO:HD2	2.39	0.52
1:A:489:ARG:HD3	5:A:2119:HOH:O	2.09	0.52
1:A:161:ALA:HA	1:A:210:SER:HB2	1.91	0.51
1:A:79:GLU:OE2	1:A:87:ALA:HB2	2.11	0.51
1:A:765:ILE:O	1:A:769:VAL:HG23	2.11	0.51
1:A:80:GLU:HG2	1:A:82:GLU:H	1.74	0.51
1:A:856:PHE:CD2	1:A:870:LEU:HD13	2.45	0.51
1:A:574:GLU:CD	1:A:574:GLU:H	2.14	0.51
1:A:762:ARG:HB3	1:A:837:TYR:HE1	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:THR:HA	1:A:357:THR:OG1	2.10	0.51
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.40	0.51
1:A:114:ASN:HB3	1:A:117:GLU:HG3	1.93	0.51
1:A:979:GLY:O	1:A:983:ILE:HG12	2.11	0.51
1:A:993:GLU:HG2	1:A:994:GLY:H	1.75	0.51
1:A:254:ASP:O	1:A:258:GLU:HB2	2.11	0.51
1:A:61:LEU:HD22	1:A:307:ILE:HG12	1.91	0.51
1:A:421:ASN:ND2	1:A:423:SER:N	2.48	0.51
1:A:899:MET:O	1:A:903:VAL:HG23	2.10	0.51
1:A:993:GLU:HG2	1:A:994:GLY:N	2.25	0.51
1:A:236:ARG:HD3	1:A:236:ARG:C	2.31	0.51
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.46	0.51
1:A:558:THR:O	1:A:558:THR:HG22	2.12	0.50
1:A:844:VAL:HG22	1:A:907:ILE:HD13	1.93	0.50
1:A:8:SER:OG	1:A:11:GLU:HG3	2.10	0.50
1:A:39:ASN:OD1	1:A:226:THR:HB	2.10	0.50
1:A:247:THR:HG23	1:A:250:GLN:H	1.75	0.50
1:A:547:SER:O	1:A:551:GLU:HG3	2.12	0.50
1:A:783:LEU:HD12	1:A:783:LEU:H	1.77	0.50
1:A:267:ILE:O	1:A:270:ALA:HB3	2.11	0.49
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.40	0.49
1:A:795:VAL:HA	1:A:799:THR:OG1	2.11	0.49
1:A:863:PRO:O	1:A:865:VAL:N	2.42	0.49
1:A:654:THR:HA	1:A:677:ALA:O	2.12	0.49
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.94	0.49
1:A:52:LEU:O	1:A:56:GLN:HG2	2.13	0.49
1:A:865:VAL:HG13	1:A:869:GLN:CG	2.43	0.49
1:A:486:GLU:O	1:A:491:ARG:NH2	2.46	0.48
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.43	0.48
1:A:314:VAL:HG11	1:A:804:ALA:HB1	1.94	0.48
1:A:544:LYS:C	1:A:544:LYS:HD3	2.33	0.48
1:A:323:THR:HA	1:A:326:MET:HE3	1.94	0.48
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.96	0.48
1:A:867:TYR:O	1:A:871:THR:HG23	2.13	0.48
1:A:662:PRO:CG	1:A:665:GLU:HG3	2.44	0.48
1:A:397:LYS:O	1:A:398:ASN:HB2	2.13	0.48
1:A:319:LEU:HB3	1:A:336:LEU:HD22	1.94	0.48
1:A:819:ARG:HG3	1:A:820:PRO:HD2	1.94	0.48
1:A:20:GLU:HA	1:A:150:ILE:HD13	1.95	0.48
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.96	0.48
1:A:328:LYS:HE2	1:A:328:LYS:O	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:MET:SD	1:A:141:LYS:HD3	2.53	0.47
1:A:263:VAL:O	1:A:267:ILE:HG12	2.14	0.47
1:A:369:ILE:HG13	1:A:528:VAL:HG11	1.94	0.47
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.96	0.47
1:A:662:PRO:CD	1:A:665:GLU:HG3	2.43	0.47
1:A:855:TRP:HZ3	1:A:966:GLN:HG2	1.79	0.47
1:A:898:THR:O	1:A:898:THR:HG22	2.15	0.47
1:A:55:GLU:CB	1:A:58:GLU:OE1	2.62	0.47
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.47	0.47
1:A:761:ILE:O	1:A:765:ILE:HG12	2.14	0.47
1:A:377:CYS:O	1:A:544:LYS:HG3	2.14	0.47
1:A:586:GLU:O	1:A:589:THR:HB	2.15	0.47
1:A:891:PHE:C	1:A:893:ALA:H	2.18	0.47
1:A:947:ILE:HG12	1:A:947:ILE:O	2.14	0.47
1:A:52:LEU:HD13	1:A:106:VAL:HG13	1.96	0.47
1:A:807:LEU:C	1:A:809:PHE:H	2.18	0.47
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.44	0.47
1:A:947:ILE:HD11	1:A:957:PHE:CE2	2.50	0.47
1:A:151:VAL:CG1	1:A:152:GLU:N	2.78	0.47
1:A:819:ARG:CG	1:A:820:PRO:HD2	2.44	0.47
1:A:85:ILE:HG23	1:A:86:THR:HG23	1.97	0.47
1:A:366:MET:HA	1:A:596:VAL:O	2.14	0.46
1:A:854:TRP:O	1:A:859:ALA:HB2	2.15	0.46
1:A:491:ARG:NH2	1:A:584:PHE:HD1	2.13	0.46
1:A:978:ILE:HG22	1:A:978:ILE:O	2.14	0.46
1:A:487:PHE:C	1:A:487:PHE:CD1	2.88	0.46
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.49	0.46
1:A:917:SER:CB	1:A:920:GLN:HB2	2.46	0.46
1:A:922:LEU:O	1:A:927:PRO:HD3	2.16	0.46
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.96	0.46
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.44	0.46
1:A:114:ASN:HB3	1:A:117:GLU:CG	2.45	0.46
1:A:488:SER:HB3	1:A:491:ARG:HH21	1.80	0.46
1:A:65:LEU:HB2	1:A:307:ILE:HD13	1.97	0.46
1:A:90:GLU:HB2	1:A:790:VAL:CG2	2.45	0.46
1:A:898:THR:OG1	1:A:959:LEU:HA	2.15	0.46
1:A:383:SER:C	1:A:384:ILE:HD13	2.36	0.46
1:A:66:LEU:CD1	1:A:98:LEU:HD13	2.46	0.46
1:A:759:GLN:HA	1:A:759:GLN:OE1	2.16	0.45
1:A:880:HIS:N	1:A:881:PRO:CD	2.79	0.45
1:A:367:PHE:C	1:A:367:PHE:CD2	2.90	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:HG3	1:A:83:GLU:N	2.31	0.45
1:A:128:LYS:HD3	1:A:139:ARG:NH1	2.31	0.45
1:A:557:ASP:CB	1:A:638:ARG:HH22	2.29	0.45
1:A:198:ARG:NH1	1:A:656:ARG:HH22	2.15	0.45
1:A:329:LYS:O	1:A:330:ASN:HB2	2.16	0.45
1:A:769:VAL:O	1:A:773:VAL:HG23	2.17	0.45
1:A:264:ILE:HD11	1:A:306:ALA:HB2	1.99	0.45
1:A:865:VAL:HG12	1:A:869:GLN:HG3	1.94	0.45
1:A:242:THR:HG21	1:A:712:LYS:CG	2.40	0.44
1:A:317:THR:O	1:A:321:LEU:HG	2.17	0.44
1:A:757:MET:HA	1:A:760:PHE:CE2	2.53	0.44
1:A:59:ASP:HB3	1:A:62:VAL:CG2	2.47	0.44
1:A:737:ASP:OD2	1:A:739:ASN:HB2	2.18	0.44
1:A:947:ILE:HD11	1:A:957:PHE:CD2	2.52	0.44
1:A:494:MET:HG2	1:A:495:SER:N	2.33	0.44
1:A:557:ASP:O	1:A:558:THR:C	2.56	0.44
1:A:975:LEU:N	1:A:976:PRO:CD	2.80	0.44
1:A:262:LYS:O	1:A:266:LEU:HD23	2.17	0.44
1:A:342:LEU:HD12	1:A:733:MET:CE	2.48	0.43
1:A:79:GLU:OE2	1:A:84:THR:HA	2.18	0.43
1:A:253:LEU:HD23	4:A:1003:TG1:H301	2.00	0.43
1:A:557:ASP:HA	1:A:638:ARG:CZ	2.47	0.43
1:A:909:MET:SD	1:A:937:ILE:HG23	2.59	0.43
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.48	0.43
1:A:836:ARG:HG3	1:A:984:LEU:HB3	2.00	0.43
1:A:983:ILE:O	1:A:987:ILE:HG12	2.18	0.43
1:A:272:TRP:HA	1:A:295:TYR:OH	2.19	0.43
1:A:488:SER:HB3	1:A:491:ARG:HE	1.84	0.43
1:A:53:VAL:O	1:A:56:GLN:N	2.46	0.43
1:A:977:VAL:C	1:A:979:GLY:N	2.70	0.43
1:A:235:ILE:HG22	1:A:239:MET:CE	2.49	0.43
1:A:397:LYS:HB3	1:A:402:ILE:HG21	2.01	0.43
1:A:635:ILE:O	1:A:639:ILE:HG12	2.18	0.43
1:A:80:GLU:HG2	1:A:82:GLU:HG2	2.01	0.43
1:A:80:GLU:O	1:A:84:THR:HB	2.19	0.43
1:A:865:VAL:HG13	1:A:869:GLN:OE1	2.19	0.43
1:A:773:VAL:O	1:A:777:LEU:HG	2.19	0.42
1:A:108:GLN:HE22	1:A:316:THR:HG21	1.84	0.42
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.02	0.42
1:A:761:ILE:HG21	1:A:828:LEU:HD13	2.01	0.42
1:A:788:ILE:CG1	1:A:791:GLN:HG3	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG13	1:A:791:GLN:HG3	2.01	0.42
1:A:80:GLU:CG	1:A:82:GLU:HG2	2.49	0.42
1:A:922:LEU:HB3	1:A:927:PRO:HG3	2.00	0.42
1:A:151:VAL:HG12	1:A:152:GLU:N	2.33	0.42
1:A:18:VAL:HG22	1:A:19:SER:N	2.34	0.42
1:A:873:PHE:HB2	1:A:891:PHE:CZ	2.53	0.42
1:A:347:VAL:HG13	1:A:620:ARG:HG3	1.99	0.42
1:A:342:LEU:CD2	1:A:747:VAL:HG22	2.46	0.42
1:A:932:TRP:O	1:A:936:SER:HB2	2.20	0.42
1:A:969:MET:HE2	1:A:973:ILE:HG12	2.01	0.42
1:A:72:SER:O	1:A:91:PRO:HG3	2.19	0.42
1:A:870:LEU:O	1:A:873:PHE:HB3	2.20	0.42
1:A:134:ARG:HD3	1:A:138:GLN:HG2	2.02	0.42
1:A:379:LEU:CD1	1:A:548:VAL:HG21	2.50	0.42
1:A:389:TYR:HB3	1:A:425:LEU:HD11	2.01	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.20	0.41
1:A:99:ILE:HG22	1:A:103:ILE:CD1	2.49	0.41
1:A:300:VAL:O	1:A:304:VAL:HG23	2.19	0.41
1:A:869:GLN:HB2	1:A:883:PHE:CE1	2.55	0.41
1:A:544:LYS:O	1:A:544:LYS:HD3	2.20	0.41
1:A:763:TYR:CD2	1:A:764:LEU:HD12	2.56	0.41
1:A:795:VAL:O	1:A:799:THR:HB	2.20	0.41
1:A:840:ILE:HD11	1:A:981:ASP:HB2	2.02	0.41
1:A:99:ILE:HG22	1:A:103:ILE:HD11	2.01	0.41
1:A:328:LYS:HE2	1:A:328:LYS:CA	2.50	0.41
1:A:190:HIS:HE1	1:A:192:GLU:O	2.04	0.41
1:A:624:ILE:HG21	1:A:684:LYS:HG2	2.02	0.41
1:A:52:LEU:HD13	1:A:110:ARG:HB2	2.03	0.41
1:A:662:PRO:HG2	1:A:665:GLU:HG3	2.03	0.41
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.90	0.41
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.02	0.41
1:A:247:THR:HG22	1:A:250:GLN:CB	2.51	0.41
1:A:274:ILE:HG22	1:A:274:ILE:O	2.21	0.41
1:A:308:PRO:HG3	1:A:765:ILE:CD1	2.51	0.41
1:A:81:GLY:HA2	1:A:84:THR:CB	2.44	0.41
1:A:922:LEU:H	1:A:922:LEU:HD12	1.86	0.41
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.36	0.40
1:A:773:VAL:HG21	1:A:842:GLY:HA2	2.02	0.40
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.86	0.40
1:A:80:GLU:CD	1:A:82:GLU:HG2	2.42	0.40
1:A:487:PHE:CD1	1:A:488:SER:N	2.90	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.52	0.40
1:A:790:VAL:O	1:A:790:VAL:HG12	2.22	0.40
1:A:914:ASN:N	1:A:914:ASN:HD22	2.20	0.40
1:A:985:LYS:O	1:A:989:ARG:HG2	2.22	0.40
1:A:486:GLU:OE1	1:A:486:GLU:N	2.47	0.40
1:A:583:ARG:HH11	1:A:583:ARG:HG2	1.85	0.40
1:A:788:ILE:HD13	1:A:958:LYS:CE	2.49	0.40
1:A:986:PHE:O	1:A:990:ASN:HB2	2.22	0.40
1:A:663:LEU:CD1	1:A:663:LEU:H	2.35	0.40
1:A:663:LEU:CD1	1:A:663:LEU:N	2.84	0.40
1:A:773:VAL:CB	1:A:845:GLY:HA3	2.51	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%)	901 (91%)	77 (8%)	15 (2%)	<b>10</b> <b>14</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	857	MET
1	A	950	VAL
1	A	78	PHE
1	A	875	GLN
1	A	881	PRO
1	A	918	GLU
1	A	58	GLU
1	A	949	TYR
1	A	978	ILE
1	A	575	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	895	GLU
1	A	864	GLY
1	A	885	GLY
1	A	865	VAL
1	A	926	PRO

### 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%)	807 (96%)	33 (4%)	32	44

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	41	LEU
1	A	45	GLU
1	A	80	GLU
1	A	114	ASN
1	A	149	ASP
1	A	164	ARG
1	A	238	GLN
1	A	328	LYS
1	A	342	LEU
1	A	356	LEU
1	A	384	ILE
1	A	402	ILE
1	A	421	ASN
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	488	SER
1	A	544	LYS
1	A	560	ARG
1	A	589	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	600	LEU
1	A	631	THR
1	A	644	GLU
1	A	656	ARG
1	A	691	LEU
1	A	713	LYS
1	A	732	GLU
1	A	740	PHE
1	A	911	ASN
1	A	923	MET
1	A	975	LEU
1	A	991	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
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	421	ASN
1	A	477	GLN
1	A	510	ASN
1	A	739	ASN
1	A	768	ASN
1	A	875	GLN
1	A	911	ASN
1	A	914	ASN
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 ⓘ

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ALF	A	998	-	0,4,4	0.00	-	-		
4	TG1	A	1003	-	43,48,48	1.82	10 (23%)	44,72,72	1.81	11 (25%)

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
4	TG1	A	1003	-	-	12/33/99/99	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TG1	O4-C21	5.89	1.33	1.21
4	A	1003	TG1	C3-C4	3.49	1.54	1.50
4	A	1003	TG1	O6-C7	3.35	1.48	1.43
4	A	1003	TG1	C34-C11	3.26	1.57	1.53
4	A	1003	TG1	C9-C10	3.17	1.59	1.54
4	A	1003	TG1	C1-C5	2.81	1.55	1.51
4	A	1003	TG1	O3-C3	2.61	1.49	1.44
4	A	1003	TG1	C11-C7	2.52	1.58	1.55
4	A	1003	TG1	C9-C8	2.34	1.55	1.52
4	A	1003	TG1	C1-C2	2.28	1.58	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	C10-O9-C32	5.86	135.44	121.53
4	A	1003	TG1	O12-C12-C11	-3.72	124.55	128.28
4	A	1003	TG1	C24-C22-C21	3.33	133.96	120.78
4	A	1003	TG1	C2-O1-C13	3.27	122.97	117.53
4	A	1003	TG1	O3-C21-O4	3.16	129.34	123.32
4	A	1003	TG1	C7-C6-C5	3.05	123.21	115.41
4	A	1003	TG1	C23-C22-C21	-2.82	109.04	116.09
4	A	1003	TG1	O5-C12-O12	2.49	124.92	121.62
4	A	1003	TG1	C11-C7-C6	-2.16	98.87	103.03
4	A	1003	TG1	C8-O7-C27	2.13	121.94	117.92
4	A	1003	TG1	O4-C21-C22	-2.01	118.90	125.21

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	TG1	O3-C21-C22-C23
4	A	1003	TG1	O3-C21-C22-C24
4	A	1003	TG1	O4-C21-C22-C24
4	A	1003	TG1	O4-C21-C22-C23
4	A	1003	TG1	C14-C15-C16-C17
4	A	1003	TG1	C15-C16-C17-C18
4	A	1003	TG1	C17-C18-C19-C20
4	A	1003	TG1	C22-C21-O3-C3
4	A	1003	TG1	O1-C13-C14-C15
4	A	1003	TG1	O7-C27-C28-C29
4	A	1003	TG1	O8-C27-C28-C29
4	A	1003	TG1	O2-C13-C14-C15

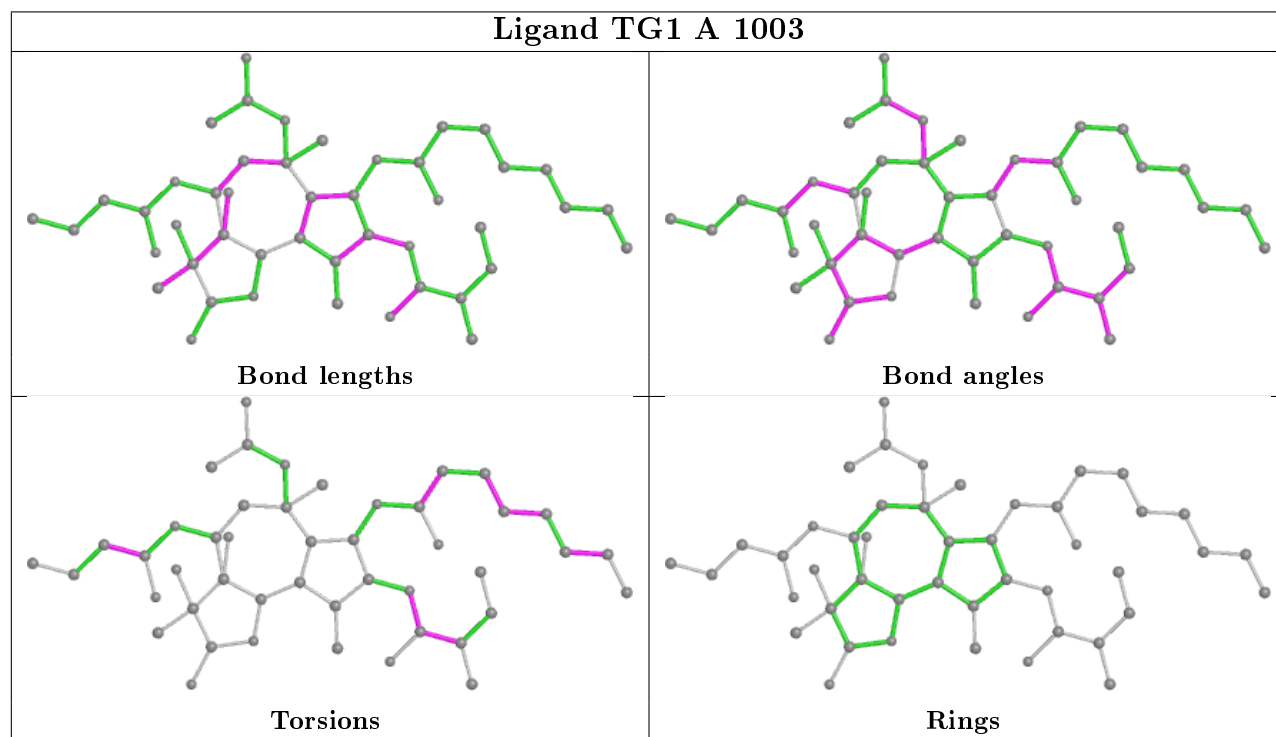
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.