



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:28 PM UTC

PDB ID : 2ZBF / pdb_00002zbf
Title : Calcium pump crystal structure with bound BeF₃ and TG in the absence of calcium
Authors : Toyoshima, C.; Ogawa, H.; Norimatsu, Y.
Deposited on : 2007-10-20
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

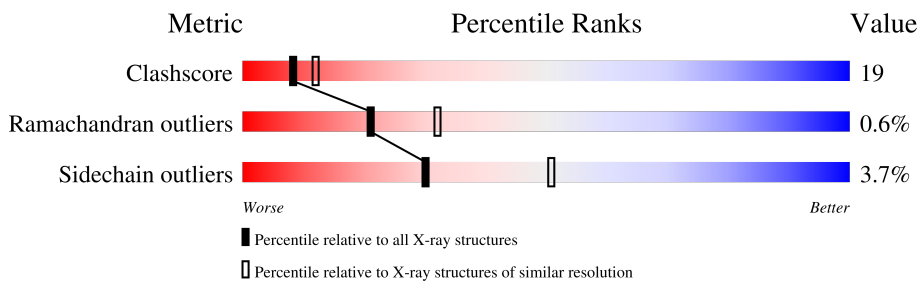
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	 64% 33% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8036 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			

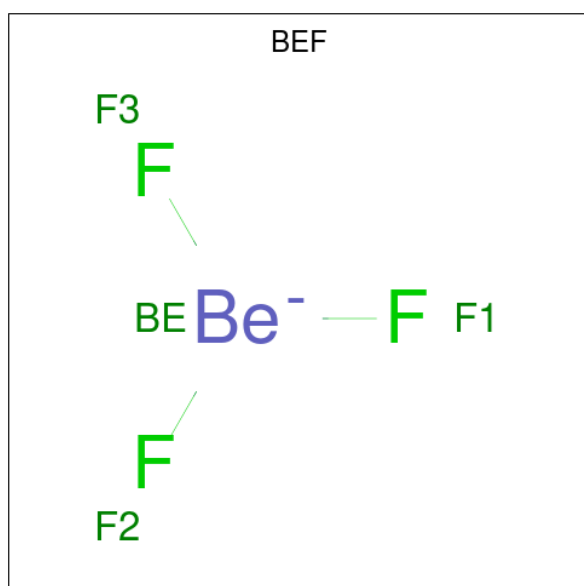
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

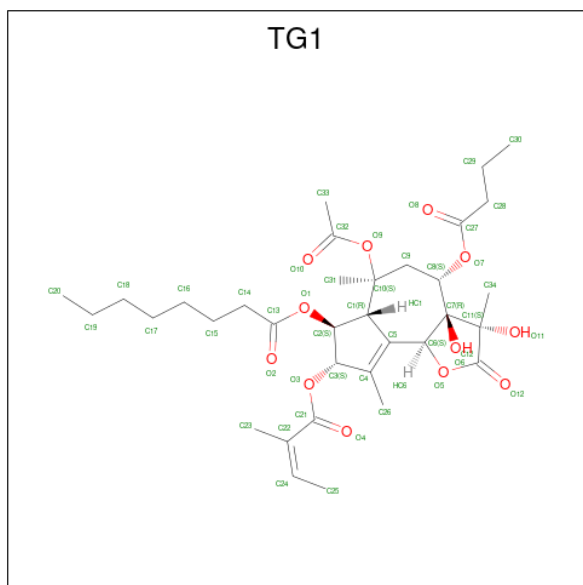
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 4 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9B]ALPHA]]-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
4	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 5 is water.

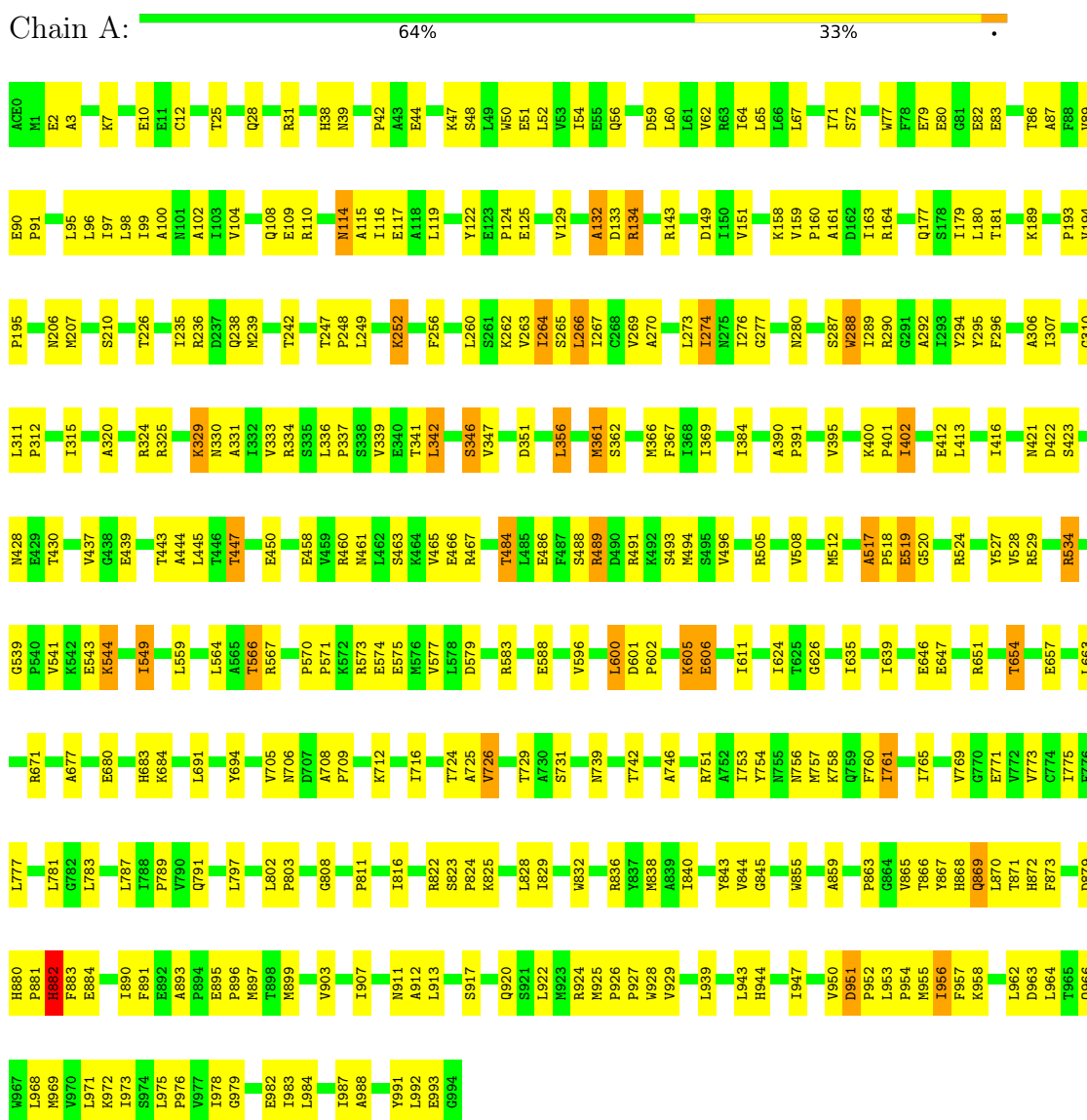
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	311	Total	O	0	0
			311	311		

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. 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	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.52Å 136.47Å 106.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 2.40	Depositor
% Data completeness (in resolution range)	94.2 (11.98-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8036	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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: MG, ACE, TG1, 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	0.47	1/7813 (0.0%)	0.92	23/10594 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	TRP	NE1-CE2	-5.51	1.31	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ILE	N-CA-C	7.11	114.94	107.76
1	A	47	LYS	O-C-N	-7.02	113.25	122.59
1	A	869	GLN	N-CA-C	-6.92	104.83	113.20
1	A	601	ASP	CA-C-N	6.50	124.34	119.66
1	A	601	ASP	C-N-CA	6.50	124.34	119.66
1	A	163	ILE	N-CA-C	6.43	118.05	108.46
1	A	925	MET	CA-C-N	6.42	127.00	120.38
1	A	925	MET	C-N-CA	6.42	127.00	120.38
1	A	517	ALA	CA-C-N	6.28	125.77	119.24
1	A	517	ALA	C-N-CA	6.28	125.77	119.24
1	A	761	ILE	N-CA-C	-6.15	104.75	110.53
1	A	912	ALA	N-CA-C	-5.93	104.90	111.36
1	A	605	LYS	N-CA-C	5.82	118.38	111.33
1	A	159	VAL	CA-C-N	5.65	125.27	119.56
1	A	159	VAL	C-N-CA	5.65	125.27	119.56
1	A	870	LEU	N-CA-C	-5.61	106.57	113.41
1	A	329	LYS	N-CA-C	-5.58	106.06	112.92
1	A	194	VAL	CA-C-N	5.56	126.79	119.84
1	A	194	VAL	C-N-CA	5.56	126.79	119.84
1	A	274	ILE	N-CA-C	-5.37	108.04	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	549	ILE	N-CA-C	-5.17	105.50	110.72
1	A	654	THR	N-CA-C	-5.13	103.16	110.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7674	0	7765	298	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	46	0	50	4	0
5	A	311	0	0	8	0
All	All	8036	0	7815	298	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 19.

All (298) 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	1.39	1.01
1:A:119:LEU:HD13	1:A:726:VAL:HG13	1.51	0.92
1:A:311:LEU:HD11	1:A:761:ILE:HD13	1.53	0.90
1:A:866:THR:H	1:A:869:GLN:HE21	1.09	0.90
1:A:600:LEU:O	1:A:602:PRO:HD3	1.72	0.89
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.54	0.87
1:A:963:ASP:HB3	1:A:966:GLN:HG3	1.54	0.86
1:A:519:GLU:CD	1:A:519:GLU:H	1.82	0.86
1:A:484:THR:HB	1:A:496:VAL:HG12	1.61	0.83
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.44	0.82
1:A:239:MET:HE2	1:A:708:ALA:HB1	1.63	0.80
1:A:838:MET:HE3	1:A:838:MET:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.66	0.78
1:A:573:ARG:H	1:A:573:ARG:HD2	1.48	0.78
1:A:781:LEU:HB3	1:A:783:LEU:HD13	1.63	0.78
1:A:421:ASN:ND2	1:A:423:SER:H	1.82	0.77
1:A:879:ASP:OD1	1:A:882:HIS:HB2	1.83	0.77
1:A:421:ASN:HD22	1:A:423:SER:H	1.32	0.76
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.68	0.76
1:A:248:PRO:HG2	5:A:2040:HOH:O	1.86	0.74
1:A:80:GLU:HG3	1:A:82:GLU:HG2	1.70	0.73
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.70	0.73
1:A:115:ALA:HA	1:A:729:THR:HG21	1.70	0.72
1:A:880:HIS:N	1:A:881:PRO:HD2	2.04	0.72
1:A:325:ARG:NH2	1:A:753:ILE:HD11	2.06	0.71
1:A:866:THR:N	1:A:869:GLN:HE21	1.85	0.71
1:A:899:MET:HE1	1:A:966:GLN:O	1.91	0.70
1:A:489:ARG:CD	1:A:489:ARG:H	2.05	0.70
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.22	0.70
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.73	0.69
1:A:769:VAL:HA	4:A:1003:TG1:H231	1.75	0.69
1:A:944:HIS:O	1:A:947:ILE:HG22	1.92	0.69
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.92	0.68
1:A:811:PRO:HG3	1:A:929:VAL:HG12	1.74	0.68
1:A:124:PRO:HG3	1:A:160:PRO:HA	1.74	0.68
1:A:97:ILE:HD13	1:A:797:LEU:HD11	1.75	0.67
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.95	0.67
1:A:783:LEU:CD1	1:A:871:THR:HG22	2.24	0.67
1:A:520:GLY:O	1:A:524:ARG:HG3	1.95	0.67
1:A:342:LEU:HD13	1:A:746:ALA:HB1	1.77	0.66
1:A:90:GLU:OE2	1:A:789:PRO:HG2	1.96	0.66
1:A:116:ILE:HD11	1:A:236:ARG:HE	1.60	0.66
1:A:880:HIS:N	1:A:881:PRO:CD	2.58	0.66
1:A:100:ALA:O	1:A:104:VAL:HG23	1.95	0.65
1:A:86:THR:HB	1:A:89:VAL:HG21	1.77	0.65
1:A:963:ASP:H	1:A:966:GLN:HE21	1.44	0.65
1:A:366:MET:HE2	1:A:384:ILE:HD11	1.77	0.65
1:A:567:ARG:NH1	1:A:571:PRO:HD3	2.12	0.65
1:A:62:VAL:HG13	1:A:98:LEU:HD22	1.78	0.64
1:A:783:LEU:HD11	1:A:871:THR:HG22	1.79	0.64
1:A:836:ARG:O	1:A:840:ILE:HG12	1.97	0.64
1:A:950:VAL:O	1:A:954:PRO:HD2	1.97	0.64
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.79	0.63
1:A:893:ALA:HB1	1:A:895:GLU:OE1	1.98	0.63
1:A:413:LEU:HG	1:A:564:LEU:HD12	1.79	0.63
1:A:320:ALA:O	1:A:324:ARG:HG2	1.99	0.62
1:A:262:LYS:O	1:A:266:LEU:HB2	2.00	0.62
1:A:44:GLU:HB2	1:A:116:ILE:HD13	1.81	0.62
1:A:567:ARG:NH1	1:A:570:PRO:HA	2.14	0.62
1:A:458:GLU:OE2	1:A:460:ARG:HG2	2.01	0.61
1:A:968:LEU:O	1:A:972:LYS:HG2	2.00	0.61
1:A:866:THR:H	1:A:869:GLN:NE2	1.90	0.61
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.82	0.61
1:A:2:GLU:O	1:A:3:ALA:HB3	2.01	0.60
1:A:310:GLY:HA2	1:A:797:LEU:HD23	1.84	0.59
1:A:488:SER:HB3	1:A:491:ARG:HH21	1.67	0.59
1:A:867:TYR:O	1:A:871:THR:HG23	2.02	0.59
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.84	0.59
1:A:606:GLU:H	1:A:606:GLU:CD	2.08	0.59
1:A:863:PRO:HD3	1:A:890:ILE:HD11	1.85	0.59
1:A:549:ILE:HD11	1:A:596:VAL:CG2	2.25	0.58
1:A:651:ARG:HH11	1:A:651:ARG:HG3	1.68	0.58
1:A:489:ARG:H	1:A:489:ARG:NE	2.01	0.58
1:A:423:SER:HB3	1:A:437:VAL:O	2.04	0.58
1:A:341:THR:HG22	1:A:716:ILE:HD11	1.85	0.58
1:A:527:TYR:HB3	1:A:534:ARG:HG3	1.85	0.57
1:A:964:LEU:C	1:A:964:LEU:HD23	2.30	0.57
1:A:367:PHE:C	1:A:367:PHE:CD2	2.82	0.57
1:A:395:VAL:O	1:A:402:ILE:HD13	2.04	0.57
1:A:288:TRP:C	1:A:289:ILE:HD12	2.29	0.57
1:A:757:MET:O	1:A:761:ILE:HG12	2.04	0.57
1:A:247:THR:HG22	1:A:249:LEU:H	1.70	0.57
1:A:573:ARG:H	1:A:573:ARG:CD	2.14	0.57
1:A:238:GLN:O	1:A:242:THR:HG23	2.06	0.56
1:A:663:LEU:H	1:A:663:LEU:CD1	2.17	0.56
1:A:52:LEU:O	1:A:56:GLN:HG2	2.04	0.56
1:A:402:ILE:HD13	1:A:402:ILE:H	1.69	0.56
1:A:725:ALA:O	1:A:729:THR:HG23	2.05	0.56
1:A:289:ILE:HD12	1:A:289:ILE:N	2.21	0.56
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.87	0.55
1:A:963:ASP:OD2	1:A:964:LEU:N	2.39	0.55
1:A:489:ARG:H	1:A:489:ARG:HD3	1.71	0.55
1:A:963:ASP:H	1:A:966:GLN:NE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HA	1:A:132:ALA:HB3	1.89	0.55
1:A:963:ASP:N	1:A:966:GLN:HE21	2.04	0.55
1:A:979:GLY:O	1:A:983:ILE:HG12	2.06	0.55
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.07	0.54
1:A:969:MET:HE2	1:A:973:ILE:HG12	1.89	0.54
1:A:463:SER:OG	1:A:465:VAL:HG22	2.07	0.54
1:A:865:VAL:HG13	1:A:869:GLN:CG	2.37	0.54
1:A:917:SER:OG	1:A:920:GLN:HB2	2.06	0.54
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.38	0.54
1:A:52:LEU:HD22	1:A:109:GLU:HG2	1.90	0.54
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.08	0.54
1:A:114:ASN:ND2	1:A:115:ALA:H	2.06	0.53
1:A:463:SER:OG	1:A:466:GLU:HG3	2.08	0.53
1:A:777:LEU:O	1:A:781:LEU:HD13	2.09	0.53
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.90	0.53
1:A:978:ILE:O	1:A:982:GLU:HB2	2.09	0.53
1:A:413:LEU:C	1:A:413:LEU:HD23	2.33	0.53
1:A:239:MET:HE2	1:A:708:ALA:CB	2.38	0.53
1:A:114:ASN:HB3	1:A:117:GLU:HB2	1.91	0.52
1:A:264:ILE:HD11	1:A:306:ALA:CB	2.40	0.52
1:A:10:GLU:H	1:A:10:GLU:CD	2.18	0.52
1:A:97:ILE:CD1	1:A:797:LEU:HD11	2.39	0.52
1:A:605:LYS:HG3	5:A:2107:HOH:O	2.10	0.52
1:A:239:MET:HE1	1:A:726:VAL:HG12	1.92	0.52
1:A:310:GLY:CA	1:A:797:LEU:HD23	2.39	0.52
1:A:67:LEU:O	1:A:71:ILE:HG13	2.10	0.52
1:A:267:ILE:HG12	4:A:1003:TG1:H202	1.92	0.51
1:A:443:THR:O	1:A:447:THR:HG23	2.10	0.51
1:A:952:PRO:O	1:A:956:ILE:HG12	2.09	0.51
1:A:829:ILE:HG21	4:A:1003:TG1:O10	2.11	0.51
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.91	0.51
1:A:28:GLN:HG2	1:A:31:ARG:HH22	1.76	0.51
1:A:59:ASP:HB3	1:A:62:VAL:HG23	1.93	0.51
1:A:421:ASN:HD22	1:A:421:ASN:C	2.19	0.51
1:A:895:GLU:CD	1:A:895:GLU:H	2.18	0.51
1:A:236:ARG:HD3	1:A:236:ARG:C	2.37	0.50
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.93	0.50
1:A:489:ARG:CD	1:A:489:ARG:N	2.74	0.50
1:A:114:ASN:HD22	1:A:115:ALA:H	1.58	0.50
1:A:179:ILE:HG23	1:A:724:THR:CG2	2.41	0.50
1:A:50:TRP:O	1:A:54:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ARG:HG3	1:A:651:ARG:NH1	2.27	0.50
1:A:964:LEU:O	1:A:968:LEU:HG	2.11	0.50
1:A:39:ASN:OD1	1:A:226:THR:HB	2.12	0.49
1:A:983:ILE:O	1:A:987:ILE:HG12	2.11	0.49
1:A:491:ARG:HD2	1:A:588:GLU:OE2	2.12	0.49
1:A:969:MET:O	1:A:973:ILE:HG12	2.11	0.49
1:A:879:ASP:C	1:A:881:PRO:HD2	2.37	0.49
1:A:362:SER:HB2	1:A:602:PRO:HG3	1.94	0.49
1:A:865:VAL:HG13	1:A:869:GLN:HG3	1.94	0.49
1:A:939:LEU:O	1:A:943:LEU:HG	2.12	0.49
1:A:754:TYR:CE2	1:A:758:LYS:HD2	2.48	0.49
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.78	0.48
1:A:624:ILE:HG22	1:A:684:LYS:HG2	1.95	0.48
1:A:724:THR:OG1	1:A:726:VAL:HG23	2.13	0.48
1:A:247:THR:HG23	1:A:248:PRO:HD2	1.95	0.48
1:A:663:LEU:HD12	1:A:663:LEU:N	2.28	0.48
1:A:663:LEU:CD1	1:A:663:LEU:N	2.77	0.48
1:A:873:PHE:HB2	1:A:891:PHE:CD2	2.49	0.48
1:A:865:VAL:HG12	1:A:866:THR:O	2.13	0.48
1:A:263:VAL:HG11	4:A:1003:TG1:O4	2.14	0.48
1:A:651:ARG:HD3	5:A:2161:HOH:O	2.13	0.48
1:A:991:TYR:CD1	1:A:991:TYR:N	2.81	0.48
1:A:868:HIS:NE2	1:A:883:PHE:CZ	2.82	0.48
1:A:783:LEU:HD12	1:A:871:THR:HG22	1.96	0.48
1:A:705:VAL:HG22	1:A:726:VAL:HG21	1.95	0.47
1:A:116:ILE:N	1:A:116:ILE:HD12	2.29	0.47
1:A:880:HIS:O	1:A:884:GLU:HA	2.14	0.47
1:A:926:PRO:O	1:A:929:VAL:HG23	2.15	0.47
1:A:48:SER:H	1:A:51:GLU:HG3	1.79	0.47
1:A:108:GLN:NE2	1:A:336:LEU:HD12	2.29	0.47
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.94	0.47
1:A:971:LEU:O	1:A:975:LEU:HD23	2.15	0.47
1:A:311:LEU:HD11	1:A:761:ILE:CD1	2.37	0.47
1:A:79:GLU:HG2	1:A:87:ALA:HB2	1.97	0.47
1:A:124:PRO:HD2	5:A:2091:HOH:O	2.14	0.47
1:A:179:ILE:HD12	5:A:2113:HOH:O	2.14	0.47
1:A:544:LYS:O	1:A:544:LYS:HD3	2.15	0.47
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.96	0.47
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.97	0.46
1:A:947:ILE:HD11	1:A:957:PHE:CG	2.50	0.46
1:A:96:LEU:C	1:A:96:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:OE1	1:A:125:GLU:HA	2.15	0.46
1:A:421:ASN:HD22	1:A:422:ASP:N	2.13	0.46
1:A:771:GLU:O	1:A:775:ILE:HG12	2.15	0.46
1:A:260:LEU:O	1:A:264:ILE:HG12	2.16	0.46
1:A:606:GLU:CD	1:A:606:GLU:N	2.74	0.46
1:A:98:LEU:O	1:A:102:ALA:HB2	2.16	0.46
1:A:72:SER:OG	1:A:91:PRO:HG3	2.16	0.45
1:A:274:ILE:O	1:A:274:ILE:HG22	2.16	0.45
1:A:161:ALA:HA	1:A:210:SER:HB2	1.99	0.45
1:A:180:LEU:O	1:A:706:ASN:HB3	2.16	0.45
1:A:880:HIS:O	1:A:884:GLU:CA	2.65	0.45
1:A:824:PRO:C	1:A:825:LYS:HE2	2.40	0.45
1:A:825:LYS:HE2	1:A:825:LYS:HA	1.98	0.45
1:A:333:VAL:HG11	1:A:339:VAL:CG2	2.47	0.45
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.98	0.45
1:A:519:GLU:CD	1:A:519:GLU:N	2.62	0.45
1:A:179:ILE:HG23	1:A:724:THR:HG21	1.97	0.45
1:A:193:PRO:O	1:A:195:PRO:HD3	2.16	0.45
1:A:351:ASP:O	1:A:356:LEU:HD22	2.17	0.45
1:A:86:THR:HB	1:A:89:VAL:CG2	2.46	0.44
1:A:179:ILE:HG22	1:A:179:ILE:O	2.17	0.44
1:A:315:ILE:HD11	1:A:761:ILE:HD11	1.99	0.44
1:A:177:GLN:HE22	1:A:189:LYS:HZ1	1.66	0.44
1:A:277:GLY:HA2	1:A:280:ASN:ND2	2.33	0.44
1:A:505:ARG:HB3	1:A:508:VAL:CG2	2.47	0.44
1:A:524:ARG:HH21	1:A:588:GLU:HB2	1.81	0.44
1:A:897:MET:HE1	1:A:958:LYS:HE3	1.98	0.44
1:A:206:ASN:OD1	1:A:207:MET:HG2	2.17	0.44
1:A:486:GLU:O	1:A:491:ARG:NH2	2.47	0.44
1:A:42:PRO:O	1:A:116:ILE:HG21	2.17	0.44
1:A:491:ARG:HG2	1:A:493:SER:OG	2.18	0.44
1:A:956:ILE:HG12	1:A:956:ILE:H	1.52	0.44
1:A:235:ILE:HG13	5:A:2110:HOH:O	2.17	0.43
1:A:494:MET:HE2	5:A:2252:HOH:O	2.18	0.43
1:A:559:LEU:CD2	1:A:600:LEU:HG	2.47	0.43
1:A:654:THR:HA	1:A:677:ALA:O	2.18	0.43
1:A:975:LEU:N	1:A:976:PRO:HD2	2.33	0.43
1:A:761:ILE:O	1:A:765:ILE:HG12	2.19	0.43
1:A:899:MET:O	1:A:903:VAL:HG23	2.19	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.87	0.43
1:A:836:ARG:HA	1:A:984:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HG2	1:A:828:LEU:HD13	1.99	0.43
1:A:465:VAL:HG23	1:A:466:GLU:N	2.33	0.43
1:A:65:LEU:HD23	1:A:98:LEU:HD21	2.00	0.43
1:A:122:TYR:CE1	1:A:179:ILE:HG21	2.53	0.43
1:A:400:LYS:HA	1:A:401:PRO:HD3	1.89	0.43
1:A:460:ARG:CZ	1:A:461:ASN:HD21	2.32	0.43
1:A:2:GLU:O	1:A:3:ALA:CB	2.66	0.43
1:A:177:GLN:HE22	1:A:189:LYS:NZ	2.17	0.43
1:A:346:SER:OG	1:A:347:VAL:HG23	2.19	0.43
1:A:512:MET:HB2	1:A:567:ARG:HB3	2.00	0.43
1:A:895:GLU:N	1:A:896:PRO:HD2	2.33	0.43
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.53	0.43
1:A:265:SER:O	1:A:269:VAL:HG23	2.18	0.43
1:A:390:ALA:HA	1:A:391:PRO:HD3	1.82	0.43
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.91	0.43
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.48	0.43
1:A:181:THR:O	1:A:626:GLY:HA3	2.19	0.43
1:A:77:TRP:C	1:A:79:GLU:H	2.27	0.43
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.01	0.43
1:A:329:LYS:O	1:A:330:ASN:HB2	2.19	0.42
1:A:951:ASP:HB2	1:A:952:PRO:HD3	2.01	0.42
1:A:60:LEU:O	1:A:64:ILE:HG13	2.18	0.42
1:A:757:MET:HA	1:A:760:PHE:CE2	2.54	0.42
1:A:38:HIS:CD2	1:A:143:ARG:NH1	2.87	0.42
1:A:577:VAL:HG12	1:A:579:ASP:OD2	2.19	0.42
1:A:44:GLU:HB3	1:A:114:ASN:HD21	1.84	0.42
1:A:48:SER:O	1:A:52:LEU:HG	2.19	0.42
1:A:334:ARG:HD3	1:A:731:SER:O	2.19	0.42
1:A:671:ARG:HD3	1:A:694:TYR:CZ	2.54	0.42
1:A:913:LEU:O	1:A:922:LEU:HD21	2.20	0.42
1:A:122:TYR:CZ	1:A:179:ILE:HG21	2.55	0.42
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.55	0.42
1:A:288:TRP:H	1:A:289:ILE:HD12	1.85	0.42
1:A:428:ASN:OD1	1:A:430:THR:HB	2.20	0.42
1:A:947:ILE:HD11	1:A:957:PHE:CD2	2.54	0.42
1:A:264:ILE:HD11	1:A:306:ALA:HB3	2.02	0.42
1:A:539:GLY:O	1:A:543:GLU:HG3	2.19	0.42
1:A:751:ARG:HB3	1:A:816:ILE:HD11	2.01	0.42
1:A:947:ILE:HD11	1:A:957:PHE:CD1	2.55	0.42
1:A:239:MET:O	1:A:712:LYS:HD3	2.20	0.41
1:A:270:ALA:O	1:A:274:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:O	1:A:295:TYR:C	2.62	0.41
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.20	0.41
1:A:781:LEU:CB	1:A:783:LEU:HD13	2.44	0.41
1:A:680:GLU:O	1:A:683:HIS:HB2	2.21	0.41
1:A:924:ARG:O	1:A:926:PRO:HD3	2.20	0.41
1:A:296:PHE:CD1	1:A:296:PHE:N	2.87	0.41
1:A:756:ASN:HB3	1:A:808:GLY:HA2	2.01	0.41
1:A:825:LYS:HE2	1:A:825:LYS:CA	2.50	0.41
1:A:391:PRO:HB3	1:A:450:GLU:HB3	2.02	0.41
1:A:7:LYS:HE3	5:A:2219:HOH:O	2.20	0.41
1:A:59:ASP:HB3	1:A:62:VAL:CG2	2.50	0.41
1:A:80:GLU:C	1:A:82:GLU:H	2.28	0.41
1:A:158:LYS:HE3	1:A:158:LYS:HB2	1.96	0.41
1:A:242:THR:O	1:A:712:LYS:HE2	2.20	0.41
1:A:402:ILE:HD13	1:A:402:ILE:N	2.35	0.41
1:A:646:GLU:HG2	1:A:647:GLU:N	2.35	0.41
1:A:868:HIS:O	1:A:872:HIS:ND1	2.48	0.41
1:A:869:GLN:OE1	1:A:883:PHE:HB3	2.21	0.41
1:A:247:THR:HG22	1:A:249:LEU:N	2.36	0.41
1:A:369:ILE:HG13	1:A:528:VAL:HG13	2.01	0.41
1:A:583:ARG:HE	1:A:583:ARG:HB3	1.75	0.41
1:A:635:ILE:O	1:A:639:ILE:HG12	2.20	0.41
1:A:110:ARG:HG3	1:A:110:ARG:NH1	2.35	0.41
1:A:333:VAL:HG11	1:A:339:VAL:HG22	2.02	0.41
1:A:361:MET:HB3	1:A:444:ALA:HB2	2.03	0.41
1:A:832:TRP:CD1	1:A:988:ALA:HB2	2.56	0.41
1:A:884:GLU:H	1:A:884:GLU:HG2	1.56	0.41
1:A:822:ARG:HD2	1:A:823:SER:O	2.20	0.41
1:A:962:LEU:HB3	1:A:966:GLN:HB2	2.03	0.41
1:A:12:CYS:SG	1:A:164:ARG:HG3	2.61	0.40
1:A:133:ASP:HB3	1:A:134:ARG:HD2	2.04	0.40
1:A:787:LEU:HA	1:A:791:GLN:OE1	2.21	0.40
1:A:82:GLU:HG3	1:A:83:GLU:N	2.36	0.40
1:A:95:LEU:O	1:A:99:ILE:HG13	2.22	0.40
1:A:273:LEU:O	1:A:274:ILE:HD13	2.22	0.40
1:A:611:ILE:CD1	1:A:639:ILE:HD12	2.51	0.40
1:A:917:SER:CB	1:A:920:GLN:HB2	2.51	0.40
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.48	0.40
1:A:549:ILE:HD13	1:A:596:VAL:HG11	2.02	0.40
1:A:600:LEU:HD13	1:A:600:LEU:C	2.47	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%)	927 (93%)	60 (6%)	6 (1%)	21	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	SER
1	A	292	ALA
1	A	882	HIS
1	A	132	ALA
1	A	951	ASP
1	A	264	ILE

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%)	809 (96%)	31 (4%)	30	51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	134	ARG
1	A	149	ASP
1	A	252	LYS
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	346	SER
1	A	356	LEU
1	A	361	MET
1	A	402	ILE
1	A	439	GLU
1	A	445	LEU
1	A	447	THR
1	A	467	ARG
1	A	484	THR
1	A	489	ARG
1	A	519	GLU
1	A	534	ARG
1	A	544	LYS
1	A	566	THR
1	A	574	GLU
1	A	575	GLU
1	A	600	LEU
1	A	606	GLU
1	A	691	LEU
1	A	726	VAL
1	A	882	HIS
1	A	911	ASN
1	A	955	MET
1	A	956	ILE
1	A	993	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	38	HIS
1	A	108	GLN
1	A	114	ASN
1	A	177	GLN
1	A	238	GLN
1	A	280	ASN
1	A	421	ASN
1	A	461	ASN
1	A	510	ASN
1	A	869	GLN
1	A	875	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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
4	TG1	A	1003	-	44,48,48	1.80	9 (20%)	47,72,72	1.85	12 (25%)
3	BEF	A	998	1	0,3,3	-	-	-		

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	-	-	8/33/99/99	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TG1	O4-C21	6.93	1.35	1.21
4	A	1003	TG1	O6-C7	3.13	1.48	1.43
4	A	1003	TG1	C9-C10	3.07	1.59	1.54
4	A	1003	TG1	C34-C11	2.96	1.57	1.53
4	A	1003	TG1	C3-C4	2.91	1.54	1.50
4	A	1003	TG1	C31-C10	2.73	1.58	1.52
4	A	1003	TG1	C1-C5	2.72	1.55	1.51
4	A	1003	TG1	C1-C2	2.52	1.58	1.54
4	A	1003	TG1	C11-C7	2.19	1.58	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	C10-O9-C32	6.10	135.66	121.36
4	A	1003	TG1	C2-O1-C13	4.71	125.26	117.59
4	A	1003	TG1	O12-C12-C11	-3.69	124.54	128.28
4	A	1003	TG1	O7-C8-C9	2.93	111.88	106.63
4	A	1003	TG1	O5-C12-O12	2.83	125.26	121.60
4	A	1003	TG1	C10-C1-C5	2.65	118.68	115.07
4	A	1003	TG1	C7-C6-C5	2.57	122.16	115.41
4	A	1003	TG1	C24-C22-C21	2.53	130.30	120.79
4	A	1003	TG1	O1-C2-C3	-2.49	105.48	110.18
4	A	1003	TG1	O3-C21-O4	2.47	128.01	123.40
4	A	1003	TG1	C23-C22-C21	-2.27	110.29	116.12
4	A	1003	TG1	C15-C14-C13	2.18	121.69	113.69

There are no chirality outliers.

All (8) torsion outliers are listed below:

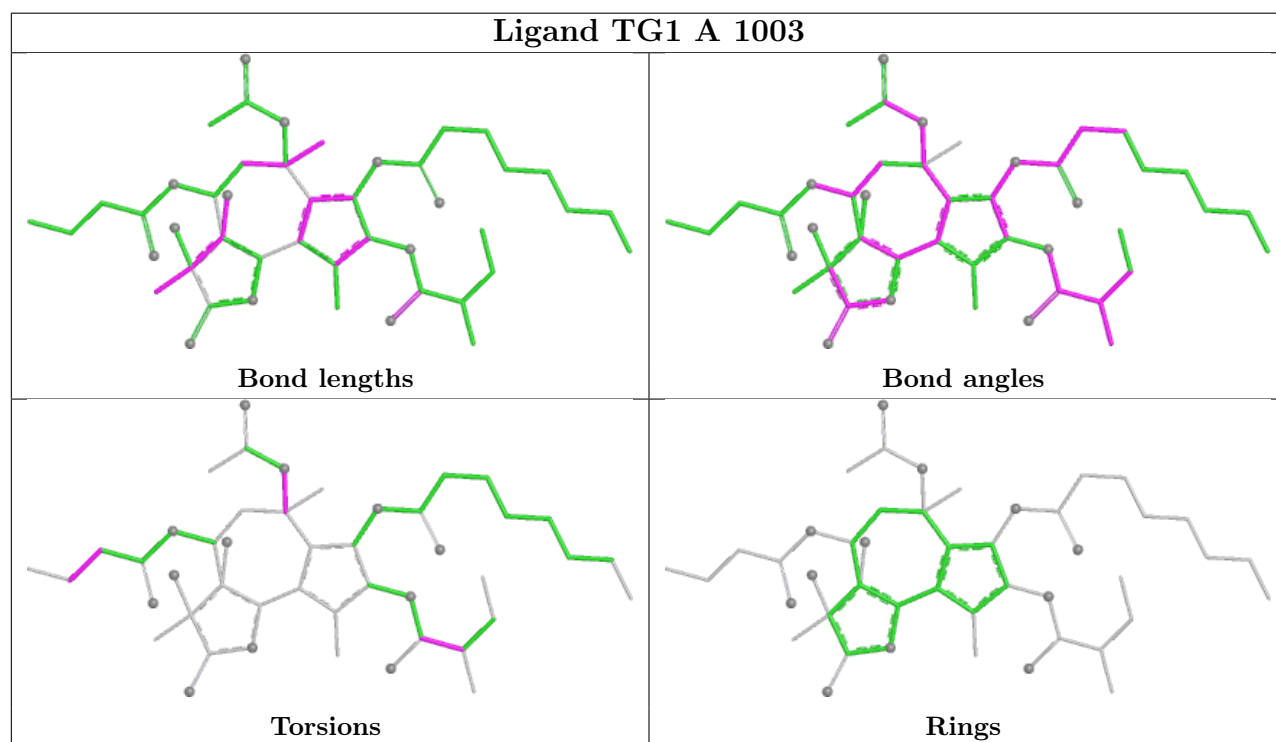
Mol	Chain	Res	Type	Atoms
4	A	1003	TG1	O3-C21-C22-C23
4	A	1003	TG1	O3-C21-C22-C24
4	A	1003	TG1	O4-C21-C22-C23
4	A	1003	TG1	C27-C28-C29-C30
4	A	1003	TG1	O4-C21-C22-C24
4	A	1003	TG1	C9-C10-O9-C32
4	A	1003	TG1	C1-C10-O9-C32
4	A	1003	TG1	C31-C10-O9-C32

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	TG1	4	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.