Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 11:47 am GMT

PDB ID	:	2ZBG
Title	:	Calcium pump crystal structure with bound AlF4 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		3.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
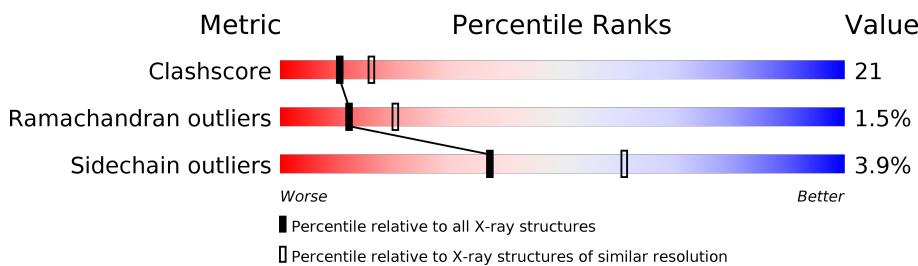
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

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

2 Entry composition ⓘ

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 7674	C 4878	N 1287	O 1452	S 57	0	0	0

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 1	Mg 1	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF$_4$).
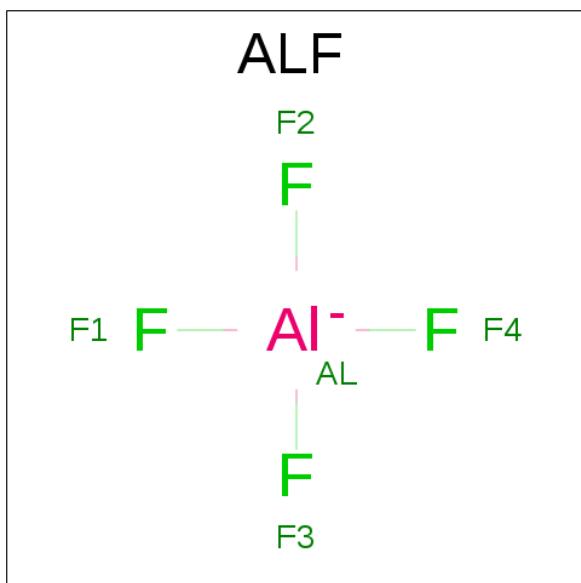
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	Al 1	F 4	0	0

- Molecule 4 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: $C_{34}H_{50}O_{12}$).
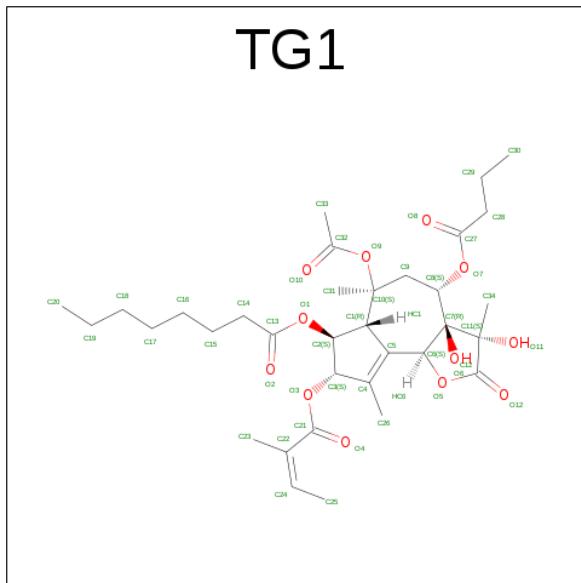
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 46	C 34	O 12	0	0

- Molecule 5 is water.

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

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.

Note EDS was not executed.

• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A:
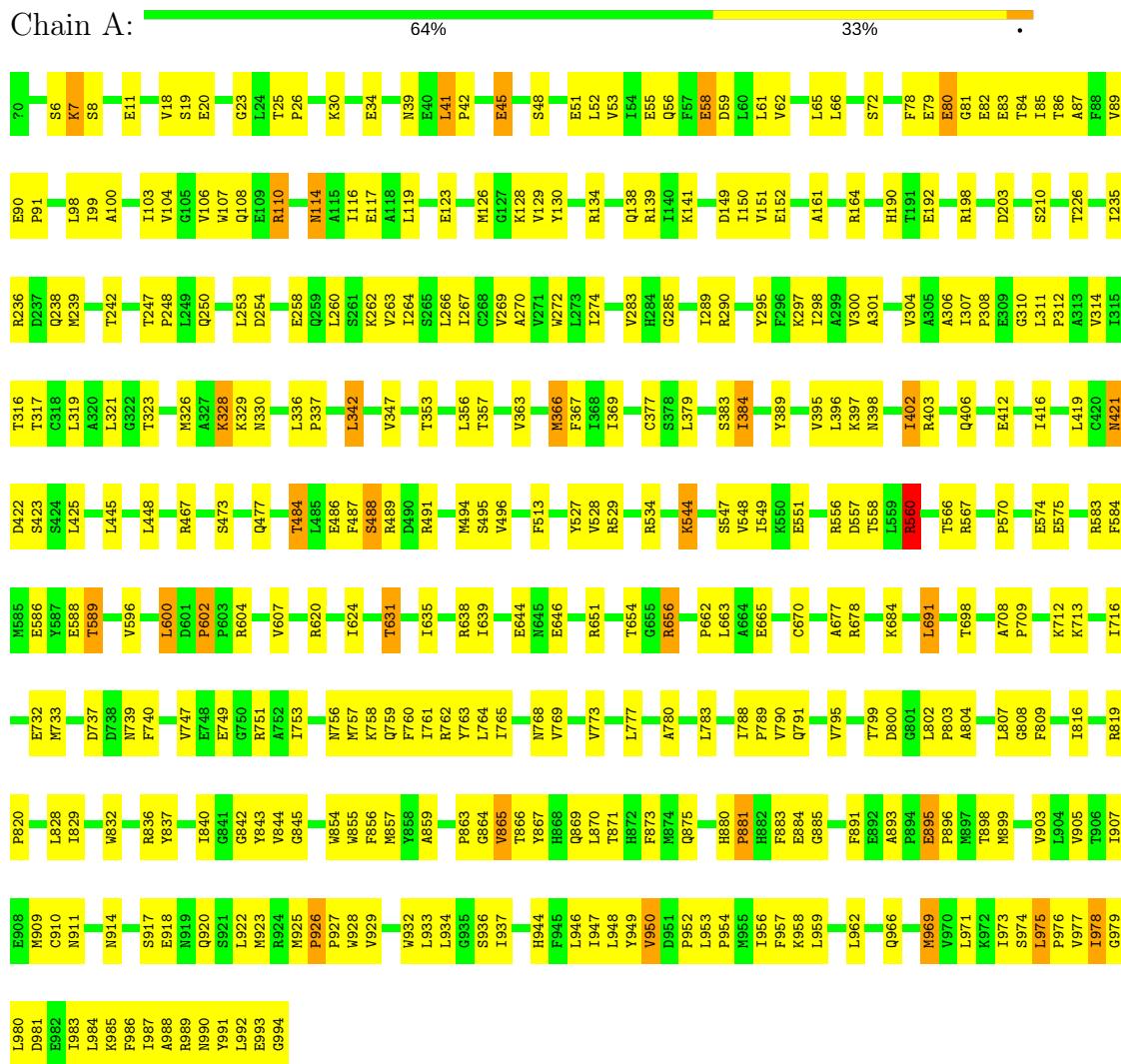
4 Data and refinement statistics ⓘ

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, α, β, γ	177.50Å 70.20Å 143.40Å 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^2)	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(^{o})	Ideal(^{o})
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 (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	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

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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

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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

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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

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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

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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

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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

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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

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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 ⓘ

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%)	901 (91%)	77 (8%)	15 (2%)	12	20

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

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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%)	37	61

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

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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	#$|Z| > 2$
4	TG1	A	1003	-	43,48,48	2.10	11 (25%)	47,72,72	1.74	9 (19%)
3	ALF	A	998	-	0,4,4	0.00	-	0,6,6	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
4	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
3	ALF	A	998	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TG1	C1-C2	2.16	1.58	1.54
4	A	1003	TG1	O3-C3	2.52	1.49	1.44
4	A	1003	TG1	C1-C5	2.72	1.55	1.51
4	A	1003	TG1	C11-C7	2.77	1.58	1.55
4	A	1003	TG1	C9-C10	2.92	1.59	1.54
4	A	1003	TG1	C9-C8	3.04	1.55	1.52
4	A	1003	TG1	C34-C11	3.10	1.57	1.53
4	A	1003	TG1	C7-C6	3.28	1.59	1.54
4	A	1003	TG1	O6-C7	3.31	1.48	1.43
4	A	1003	TG1	O4-C21	5.77	1.33	1.21
4	A	1003	TG1	C7-C8	7.42	1.63	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	O12-C12-C11	-3.93	124.55	128.28
4	A	1003	TG1	O9-C10-C31	-3.56	93.59	107.88
4	A	1003	TG1	C23-C22-C21	-2.70	109.04	116.01
4	A	1003	TG1	O5-C12-O12	2.38	124.92	121.63
4	A	1003	TG1	O3-C21-O4	3.02	129.34	123.31
4	A	1003	TG1	C24-C22-C21	3.08	133.96	120.74
4	A	1003	TG1	C2-O1-C13	3.14	122.97	117.62
4	A	1003	TG1	C7-C6-C5	3.21	123.21	114.92
4	A	1003	TG1	C10-O9-C32	5.40	135.44	121.83

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.