



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 AM UTC

PDB ID : 2O9J / pdb_00002o9j
Title : Crystal structure of calcium atpase with bound magnesium fluoride and cyclopiazonic acid
Authors : Young, H.S.; Moncoq, K.A.
Deposited on : 2006-12-13
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

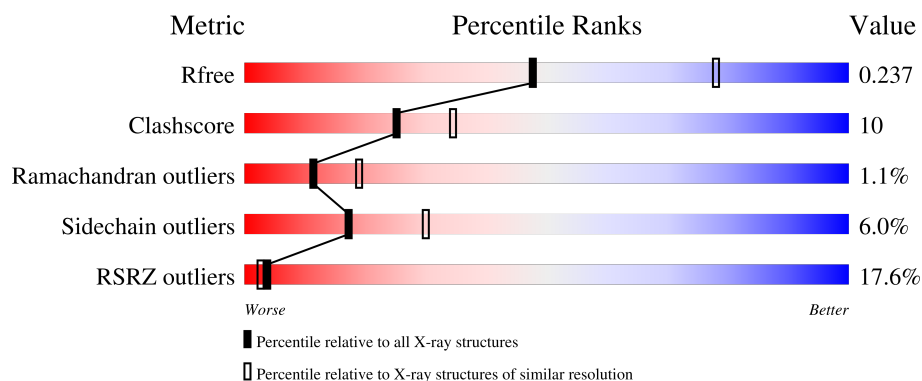
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	994	17% 77% 19% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CZA	A	1001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7669 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	980	Total	C	N	O	S	0	0	0
			7562	4805	1267	1433	57			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	variant	UNP P04191

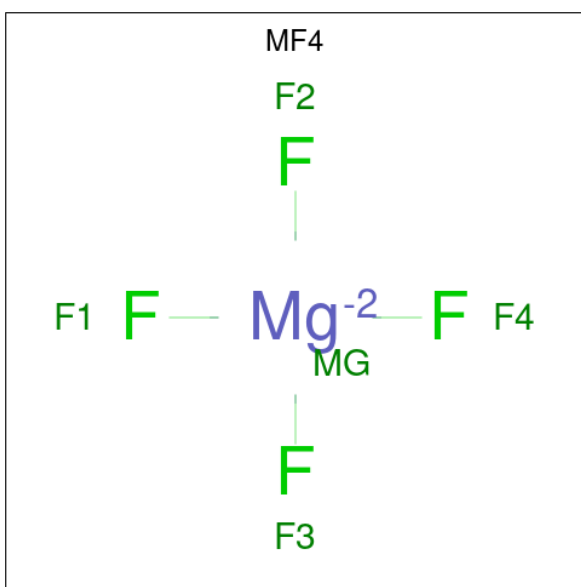
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

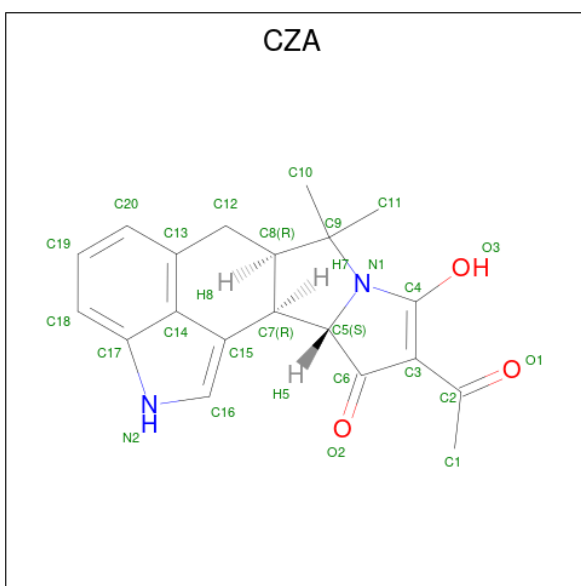
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F₄Mg).



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

- Molecule 5 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (CCD ID: CZA) (formula: C₂₀H₂₀N₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	O	
			25	20	2	3	0

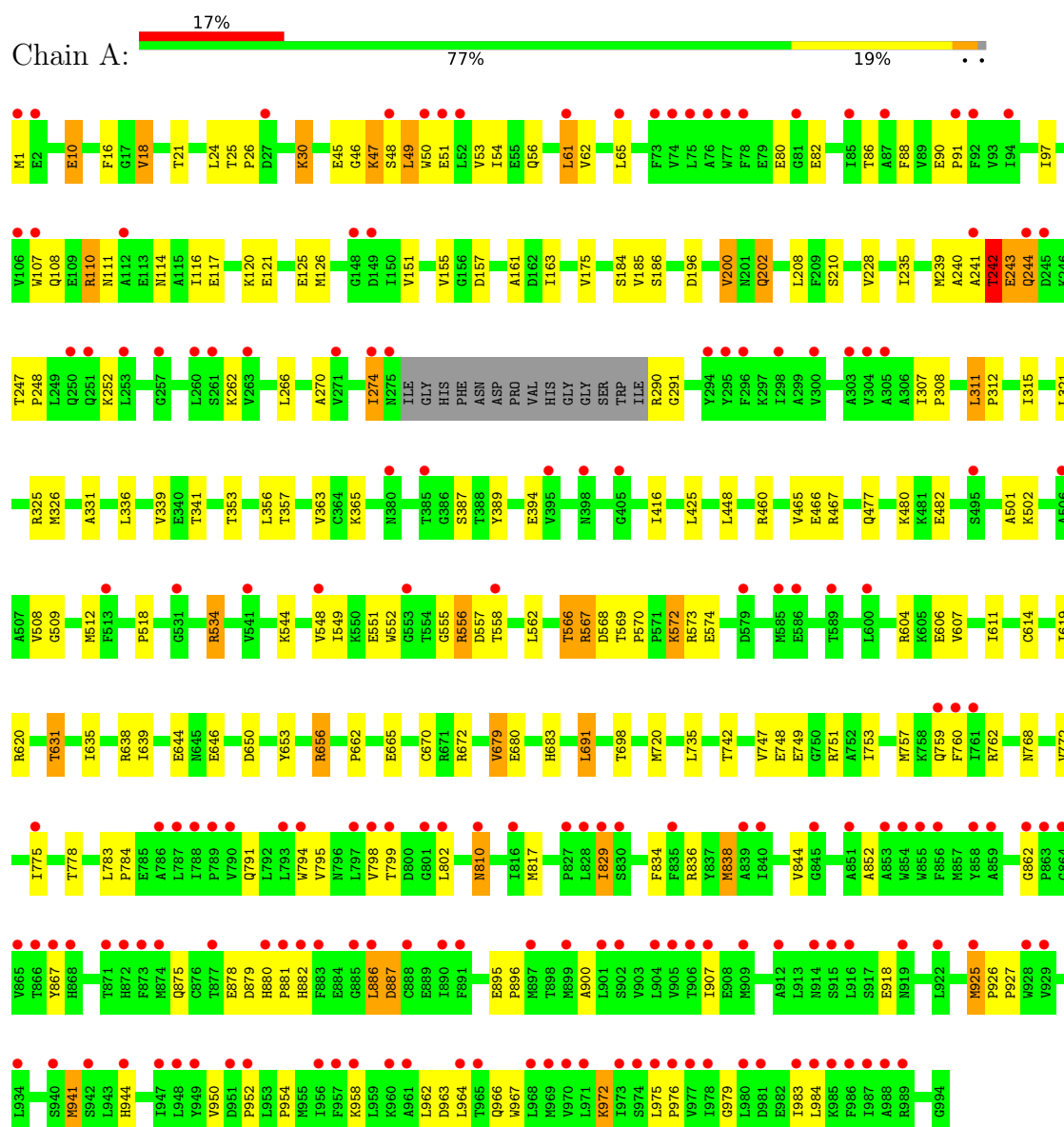
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total 75	O 75	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.38Å 69.88Å 143.41Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	29.10 – 2.65 29.10 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.10-2.65) 99.6 (29.10-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.287 0.240 , 0.237	Depositor DCC
R_{free} test set	2458 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CZA, MF4, NA

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	0.44	0/7696	0.84	5/10431 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	THR	N-CA-C	5.48	117.69	111.11
1	A	274	ILE	N-CA-C	-5.31	107.66	112.12
1	A	556	ARG	N-CA-C	-5.14	106.69	113.17
1	A	925	MET	CA-C-N	5.03	125.56	120.38
1	A	925	MET	C-N-CA	5.03	125.56	120.38

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	7562	0	7668	148	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	25	0	20	9	0
6	A	75	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7669	0	7688	148	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (148) 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:290:ARG:HD2	1:A:291:GLY:H	1.11	1.06
1:A:202:GLN:H	1:A:202:GLN:HE21	1.04	0.98
1:A:290:ARG:CD	1:A:291:GLY:H	1.83	0.91
1:A:202:GLN:HE21	1:A:202:GLN:N	1.71	0.88
1:A:720:MET:HE1	1:A:735:LEU:HD12	1.55	0.85
1:A:631:THR:HG21	6:A:2070:HOH:O	1.77	0.84
1:A:795:VAL:HA	1:A:799:THR:HG22	1.58	0.84
1:A:290:ARG:HD2	1:A:291:GLY:N	1.91	0.83
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.60	0.82
1:A:460:ARG:HD2	6:A:2050:HOH:O	1.85	0.75
1:A:751:ARG:HD2	1:A:817:MET:CE	2.17	0.74
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.70	0.73
1:A:18:VAL:CG1	1:A:24:LEU:HD23	2.20	0.72
1:A:941:MET:HE3	1:A:941:MET:HA	1.72	0.71
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.22	0.70
1:A:202:GLN:H	1:A:202:GLN:NE2	1.86	0.70
1:A:775:ILE:HA	1:A:778:THR:HG22	1.73	0.69
1:A:312:PRO:CG	5:A:1001:CZA:H112	2.23	0.68
1:A:311:LEU:HD22	1:A:315:ILE:HG13	1.75	0.67
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.76	0.67
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.76	0.66
1:A:880:HIS:N	1:A:881:PRO:HD2	2.10	0.66
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.76	0.66
1:A:555:GLY:N	6:A:2036:HOH:O	2.22	0.65
1:A:312:PRO:CD	5:A:1001:CZA:C11	2.75	0.65
1:A:312:PRO:CD	5:A:1001:CZA:H112	2.27	0.64
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.81	0.63
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.82	0.62
1:A:108:GLN:HB2	1:A:336:LEU:HB2	1.82	0.61
1:A:1:MET:HE2	1:A:16:PHE:CE1	2.34	0.61
1:A:61:LEU:HD12	5:A:1001:CZA:H8	1.84	0.60
1:A:321:LEU:O	1:A:325:ARG:HB2	2.02	0.60
1:A:950:VAL:O	1:A:954:PRO:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.84	0.58
1:A:1:MET:HE2	1:A:16:PHE:HE1	1.68	0.58
1:A:18:VAL:HG11	1:A:24:LEU:HD23	1.86	0.58
1:A:875:GLN:HB3	1:A:879:ASP:HB2	1.85	0.57
1:A:963:ASP:H	1:A:966:GLN:HG3	1.69	0.57
1:A:834:PHE:O	1:A:838:MET:HB2	2.05	0.57
1:A:880:HIS:N	1:A:881:PRO:CD	2.68	0.57
1:A:336:LEU:O	1:A:339:VAL:HG12	2.04	0.57
1:A:501:ALA:O	1:A:502:LYS:HB2	2.05	0.57
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.85	0.57
1:A:653:TYR:OH	1:A:672:ARG:NH2	2.38	0.56
1:A:312:PRO:CG	5:A:1001:CZA:C11	2.83	0.56
1:A:312:PRO:HG2	5:A:1001:CZA:C11	2.36	0.56
1:A:61:LEU:HD11	1:A:307:ILE:HD12	1.89	0.55
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.88	0.55
1:A:817:MET:HA	1:A:817:MET:HE2	1.89	0.55
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.90	0.54
1:A:247:THR:HB	1:A:248:PRO:HD2	1.90	0.54
1:A:829:ILE:HD12	1:A:829:ILE:O	2.08	0.54
1:A:241:ALA:C	1:A:243:GLU:H	2.15	0.54
1:A:574:GLU:CD	1:A:574:GLU:H	2.15	0.53
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.90	0.53
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.91	0.53
1:A:62:VAL:HG13	5:A:1001:CZA:H7	1.91	0.53
1:A:548:VAL:HA	1:A:551:GLU:HG2	1.91	0.53
1:A:312:PRO:HG2	5:A:1001:CZA:H111	1.92	0.52
1:A:326:MET:HG3	1:A:331:ALA:HB3	1.91	0.52
1:A:551:GLU:HG3	1:A:552:TRP:N	2.24	0.51
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.91	0.51
1:A:748:GLU:HA	1:A:817:MET:HE3	1.93	0.51
1:A:962:LEU:HB3	1:A:966:GLN:HB3	1.90	0.51
1:A:18:VAL:HG13	1:A:24:LEU:HD23	1.92	0.51
1:A:607:VAL:O	1:A:611:ILE:HG12	2.11	0.51
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.25	0.50
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.93	0.50
1:A:944:HIS:HE1	1:A:967:TRP:HH2	1.60	0.50
1:A:508:VAL:CG1	1:A:509:GLY:N	2.74	0.50
1:A:114:ASN:O	1:A:117:GLU:HG3	2.12	0.49
1:A:48:SER:C	1:A:50:TRP:H	2.19	0.49
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.13	0.49
1:A:508:VAL:HG12	1:A:509:GLY:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HA	6:A:2008:HOH:O	2.13	0.49
1:A:567:ARG:HD3	1:A:569:THR:O	2.12	0.49
1:A:768:ASN:O	1:A:772:VAL:HG23	2.12	0.49
1:A:46:GLY:O	1:A:47:LYS:O	2.31	0.48
1:A:312:PRO:HD3	5:A:1001:CZA:H112	1.95	0.48
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.95	0.48
1:A:290:ARG:CD	1:A:291:GLY:N	2.63	0.48
1:A:895:GLU:N	1:A:896:PRO:HD2	2.28	0.47
1:A:798:VAL:O	1:A:802:LEU:HD23	2.15	0.47
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.95	0.47
1:A:482:GLU:OE2	1:A:573:ARG:NE	2.43	0.47
1:A:544:LYS:HE2	6:A:2058:HOH:O	2.14	0.47
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.49	0.47
1:A:760:PHE:C	1:A:760:PHE:CD1	2.93	0.47
1:A:638:ARG:HD3	6:A:2041:HOH:O	2.15	0.46
1:A:534:ARG:HH11	1:A:568:ASP:HB2	1.81	0.46
1:A:972:LYS:HA	1:A:972:LYS:NZ	2.31	0.46
1:A:184:SER:O	1:A:185:VAL:C	2.59	0.46
1:A:50:TRP:O	1:A:54:ILE:HG13	2.16	0.46
1:A:196:ASP:OD2	1:A:656:ARG:NE	2.49	0.45
1:A:557:ASP:HA	1:A:638:ARG:HH22	1.81	0.45
1:A:175:VAL:O	1:A:186:SER:HA	2.17	0.45
1:A:572:LYS:O	1:A:573:ARG:C	2.59	0.45
1:A:747:VAL:HG12	1:A:817:MET:HE1	1.97	0.45
1:A:30:LYS:HA	1:A:30:LYS:HD2	1.72	0.45
1:A:944:HIS:CE1	1:A:967:TRP:HH2	2.35	0.45
1:A:572:LYS:HB3	1:A:574:GLU:OE1	2.16	0.45
1:A:353:THR:HA	1:A:357:THR:OG1	2.17	0.44
1:A:116:ILE:CD1	1:A:239:MET:HB2	2.48	0.44
1:A:836:ARG:HG3	1:A:984:LEU:HD13	1.99	0.44
1:A:979:GLY:O	1:A:983:ILE:HG12	2.18	0.44
1:A:116:ILE:HD11	1:A:239:MET:HB2	1.99	0.44
1:A:200:VAL:HG22	1:A:680:GLU:CG	2.48	0.43
1:A:242:THR:O	1:A:244:GLN:N	2.51	0.43
1:A:795:VAL:CA	1:A:799:THR:HG22	2.39	0.43
1:A:161:ALA:HA	1:A:210:SER:HB2	2.00	0.43
1:A:25:THR:HB	1:A:26:PRO:HD2	2.00	0.43
1:A:556:ARG:NH2	1:A:644:GLU:OE2	2.44	0.43
1:A:635:ILE:O	1:A:639:ILE:HG12	2.18	0.43
1:A:762:ARG:HH22	1:A:918:GLU:HG3	1.83	0.43
1:A:557:ASP:HB2	6:A:2036:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PRO:HG2	1:A:665:GLU:HG3	1.99	0.43
1:A:886:LEU:HB2	1:A:887:ASP:H	1.56	0.43
1:A:10:GLU:H	1:A:10:GLU:CD	2.27	0.43
1:A:650:ASP:O	1:A:672:ARG:HD2	2.19	0.43
1:A:757:MET:HA	1:A:760:PHE:CE2	2.54	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.82	0.43
1:A:810:ASN:ND2	1:A:810:ASN:C	2.77	0.42
1:A:270:ALA:O	1:A:274:ILE:HG13	2.19	0.42
1:A:795:VAL:HA	1:A:799:THR:CG2	2.38	0.42
1:A:116:ILE:O	1:A:120:LYS:HG3	2.20	0.42
1:A:252:LYS:HA	1:A:252:LYS:HD3	1.83	0.42
1:A:241:ALA:O	1:A:243:GLU:N	2.51	0.42
1:A:107:TRP:O	1:A:110:ARG:HD3	2.19	0.42
1:A:163:ILE:HB	1:A:208:LEU:HB2	2.01	0.42
1:A:925:MET:HA	1:A:926:PRO:HD2	1.77	0.42
1:A:97:ILE:HD13	1:A:97:ILE:HA	1.89	0.41
1:A:556:ARG:HD3	1:A:638:ARG:HG3	2.01	0.41
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.85	0.41
1:A:614:CYS:HB3	1:A:619:ILE:HB	2.03	0.41
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.02	0.41
1:A:975:LEU:N	1:A:976:PRO:HD2	2.36	0.41
1:A:791:GLN:O	1:A:795:VAL:HG23	2.21	0.41
1:A:53:VAL:O	1:A:56:GLN:HB2	2.21	0.41
1:A:110:ARG:HE	1:A:110:ARG:HB2	1.68	0.41
1:A:783:LEU:HB3	1:A:784:PRO:HD2	2.02	0.41
1:A:794:TRP:CZ3	1:A:799:THR:HB	2.56	0.41
1:A:875:GLN:HA	1:A:878:GLU:HB3	2.03	0.41
1:A:88:PHE:O	1:A:91:PRO:HD2	2.20	0.41
1:A:240:ALA:C	1:A:242:THR:H	2.28	0.40
1:A:557:ASP:O	1:A:558:THR:C	2.63	0.40
1:A:235:ILE:O	1:A:239:MET:HG2	2.21	0.40
1:A:749:GLU:O	1:A:753:ILE:HG12	2.22	0.40
1:A:80:GLU:C	1:A:82:GLU:H	2.29	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	976/994 (98%)	897 (92%)	68 (7%)	11 (1%)	11	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	111	ASN
1	A	243	GLU
1	A	862	GLY
1	A	887	ASP
1	A	49	LEU
1	A	242	THR
1	A	155	VAL
1	A	244	GLN
1	A	958	LYS
1	A	882	HIS

5.3.2 Protein sidechains [i](#)

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	829/840 (99%)	779 (94%)	50 (6%)	17	30

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	18	VAL
1	A	21	THR
1	A	30	LYS
1	A	45	GLU
1	A	49	LEU
1	A	51	GLU
1	A	61	LEU
1	A	65	LEU
1	A	86	THR
1	A	110	ARG
1	A	121	GLU
1	A	125	GLU
1	A	126	MET
1	A	151	VAL
1	A	200	VAL
1	A	202	GLN
1	A	228	VAL
1	A	242	THR
1	A	266	LEU
1	A	311	LEU
1	A	356	LEU
1	A	387	SER
1	A	394	GLU
1	A	465	VAL
1	A	466	GLU
1	A	467	ARG
1	A	477	GLN
1	A	480	LYS
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	572	LYS
1	A	606	GLU
1	A	620	ARG
1	A	631	THR
1	A	646	GLU
1	A	656	ARG
1	A	679	VAL
1	A	691	LEU
1	A	759	GLN
1	A	810	ASN

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Mol	Chain	Res	Type
1	A	829	ILE
1	A	838	MET
1	A	867	TYR
1	A	886	LEU
1	A	941	MET
1	A	964	LEU
1	A	972	LYS

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	32	HIS
1	A	38	HIS
1	A	108	GLN
1	A	114	ASN
1	A	138	GLN
1	A	202	GLN
1	A	238	GLN
1	A	359	ASN
1	A	360	GLN
1	A	472	ASN
1	A	477	GLN
1	A	755	ASN
1	A	914	ASN
1	A	944	HIS
1	A	966	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are 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	MF4	A	996	2,1	0,4,4	-	-	-		
5	CZA	A	1001	-	28,29,29	2.30	6 (21%)	29,48,48	4.55	10 (34%)

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	CZA	A	1001	-	-	4/4/52/52	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	CZA	O3-C4	5.78	1.48	1.31
5	A	1001	CZA	C4-N1	-5.48	1.34	1.39
5	A	1001	CZA	C14-C15	-4.56	1.35	1.43
5	A	1001	CZA	C3-C4	4.36	1.48	1.40
5	A	1001	CZA	O2-C6	4.10	1.29	1.22
5	A	1001	CZA	C7-C15	-2.72	1.48	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	CZA	C6-C5-N1	-15.64	92.08	103.20
5	A	1001	CZA	C5-N1-C4	11.93	123.02	111.71
5	A	1001	CZA	C14-C15-C16	8.81	112.59	106.31
5	A	1001	CZA	C15-C16-N2	-8.54	103.38	110.31
5	A	1001	CZA	O2-C6-C3	-3.58	120.04	128.42
5	A	1001	CZA	C13-C14-C15	2.90	131.34	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	CZA	C18-C17-N2	2.32	134.45	130.74
5	A	1001	CZA	C17-C14-C15	-2.17	105.13	107.59
5	A	1001	CZA	C17-N2-C16	2.06	110.91	109.08
5	A	1001	CZA	C7-C5-C6	2.05	124.92	117.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

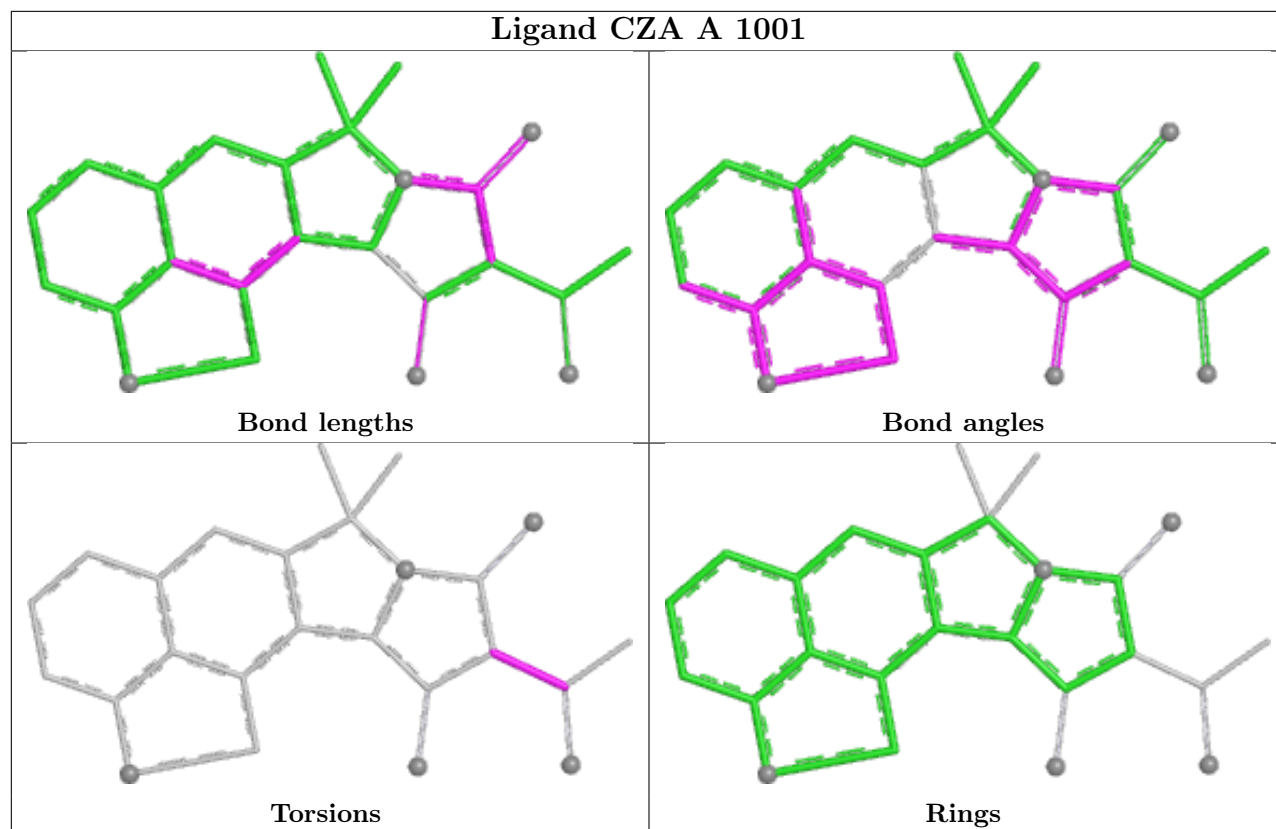
Mol	Chain	Res	Type	Atoms
5	A	1001	CZA	C1-C2-C3-C6
5	A	1001	CZA	O1-C2-C3-C4
5	A	1001	CZA	C1-C2-C3-C4
5	A	1001	CZA	O1-C2-C3-C6

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	CZA	9	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	980/994 (98%)	1.08	172 (17%) 4 3	38, 64, 145, 164	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	VAL	5.9
1	A	890	ILE	5.9
1	A	906	THR	5.5
1	A	835	PHE	5.3
1	A	905	VAL	5.2
1	A	862	GLY	5.1
1	A	886	LEU	4.9
1	A	261	SER	4.6
1	A	885	GLY	4.6
1	A	855	TRP	4.4
1	A	977	VAL	4.3
1	A	957	PHE	4.2
1	A	863	PRO	4.2
1	A	558	THR	4.2
1	A	948	LEU	4.2
1	A	75	LEU	4.1
1	A	48	SER	3.9
1	A	904	LEU	3.9
1	A	983	ILE	3.9
1	A	974	SER	3.9
1	A	978	ILE	3.8
1	A	298	ILE	3.8
1	A	854	TRP	3.7
1	A	295	TYR	3.7
1	A	973	ILE	3.7
1	A	856	PHE	3.7
1	A	899	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	3.7
1	A	50	TRP	3.5
1	A	907	ILE	3.5
1	A	877	THR	3.5
1	A	968	LEU	3.5
1	A	112	ALA	3.5
1	A	241	ALA	3.4
1	A	881	PRO	3.4
1	A	912	ALA	3.4
1	A	274	ILE	3.4
1	A	77	TRP	3.4
1	A	873	PHE	3.4
1	A	759	GLN	3.3
1	A	901	LEU	3.3
1	A	980	LEU	3.2
1	A	275	ASN	3.2
1	A	960	LYS	3.2
1	A	85	ILE	3.2
1	A	984	LEU	3.1
1	A	897	MET	3.1
1	A	816	ILE	3.1
1	A	830	SER	3.1
1	A	872	HIS	3.0
1	A	304	VAL	3.0
1	A	761	ILE	3.0
1	A	969	MET	3.0
1	A	970	VAL	3.0
1	A	858	TYR	3.0
1	A	922	LEU	3.0
1	A	951	ASP	3.0
1	A	810	ASN	2.9
1	A	981	ASP	2.9
1	A	788	ILE	2.9
1	A	975	LEU	2.9
1	A	107	TRP	2.9
1	A	585	MET	2.9
1	A	786	ALA	2.9
1	A	65	LEU	2.9
1	A	244	GLN	2.8
1	A	251	GLN	2.8
1	A	916	LEU	2.8
1	A	985	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	305	ALA	2.8
1	A	874	MET	2.8
1	A	797	LEU	2.8
1	A	271	VAL	2.7
1	A	929	VAL	2.7
1	A	880	HIS	2.7
1	A	149	ASP	2.7
1	A	883	PHE	2.7
1	A	866	THR	2.7
1	A	909	MET	2.7
1	A	27	ASP	2.7
1	A	867	TYR	2.6
1	A	253	LEU	2.6
1	A	794	TRP	2.6
1	A	73	PHE	2.6
1	A	865	VAL	2.6
1	A	864	GLY	2.6
1	A	61	LEU	2.6
1	A	257	GLY	2.6
1	A	793	LEU	2.6
1	A	914	ASN	2.6
1	A	787	LEU	2.5
1	A	802	LEU	2.5
1	A	971	LEU	2.5
1	A	531	GLY	2.5
1	A	553	GLY	2.5
1	A	801	GLY	2.5
1	A	398	ASN	2.5
1	A	919	ASN	2.5
1	A	260	LEU	2.5
1	A	600	LEU	2.5
1	A	263	VAL	2.5
1	A	380	ASN	2.5
1	A	902	SER	2.5
1	A	52	LEU	2.5
1	A	586	GLU	2.5
1	A	405	GLY	2.5
1	A	541	VAL	2.5
1	A	853	ALA	2.5
1	A	965	THR	2.5
1	A	940	SER	2.5
1	A	51	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	2.5
1	A	891	PHE	2.5
1	A	961	ALA	2.5
1	A	958	LYS	2.4
1	A	840	ILE	2.4
1	A	882	HIS	2.4
1	A	2	GLU	2.4
1	A	106	VAL	2.4
1	A	944	HIS	2.4
1	A	300	VAL	2.4
1	A	798	VAL	2.4
1	A	775	ILE	2.4
1	A	942	SER	2.4
1	A	952	PRO	2.4
1	A	851	ALA	2.4
1	A	871	THR	2.3
1	A	928	TRP	2.3
1	A	148	GLY	2.3
1	A	250	GLN	2.3
1	A	78	PHE	2.3
1	A	956	ILE	2.3
1	A	395	VAL	2.3
1	A	799	THR	2.3
1	A	845	GLY	2.3
1	A	790	VAL	2.3
1	A	92	PHE	2.3
1	A	296	PHE	2.3
1	A	829	ILE	2.2
1	A	947	ILE	2.2
1	A	989	ARG	2.2
1	A	495	SER	2.2
1	A	915	SER	2.2
1	A	760	PHE	2.2
1	A	859	ALA	2.2
1	A	934	LEU	2.2
1	A	964	LEU	2.2
1	A	986	PHE	2.2
1	A	506	ALA	2.2
1	A	988	ALA	2.2
1	A	87	ALA	2.2
1	A	303	ALA	2.2
1	A	589	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	888	CYS	2.2
1	A	548	VAL	2.2
1	A	868	HIS	2.2
1	A	91	PRO	2.1
1	A	789	PRO	2.1
1	A	949	TYR	2.1
1	A	81	GLY	2.1
1	A	976	PRO	2.1
1	A	925	MET	2.1
1	A	987	ILE	2.1
1	A	385	THR	2.1
1	A	94	ILE	2.1
1	A	579	ASP	2.1
1	A	827	PRO	2.1
1	A	1	MET	2.1
1	A	513	PHE	2.0
1	A	245	ASP	2.0
1	A	839	ALA	2.0
1	A	828	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

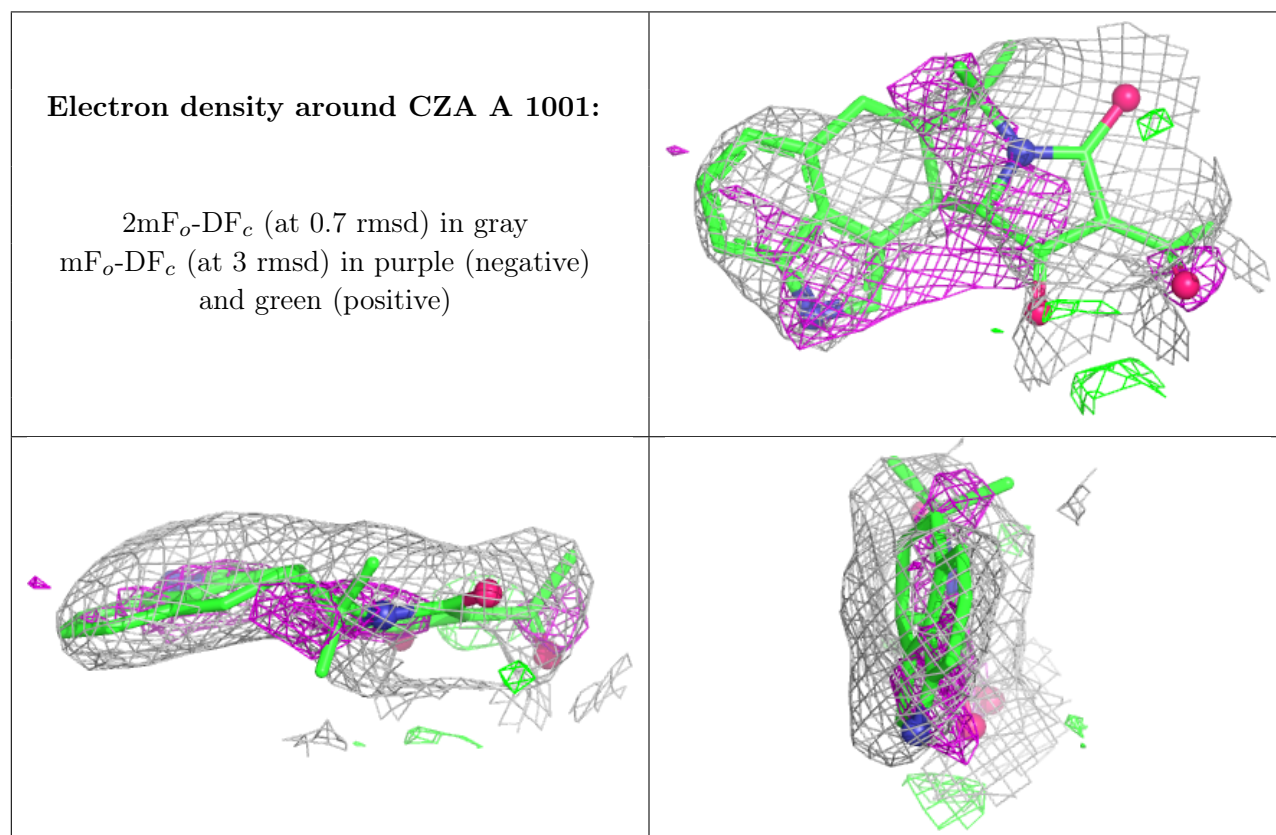
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CZA	A	1001	25/25	0.73	0.20	89,89,91,92	0
3	NA	A	997	1/1	0.84	0.16	48,48,48,48	0
4	MF4	A	996	5/5	0.93	0.11	32,34,35,35	0
2	MG	A	995	1/1	1.00	0.08	36,36,36,36	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.