



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 06:24 AM EDT

PDB ID : 10ZF / pdb_000010zf
Title : Structure of c-Cbl bound to compound 33
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Deposited on : 2026-02-12
Resolution : 2.39 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

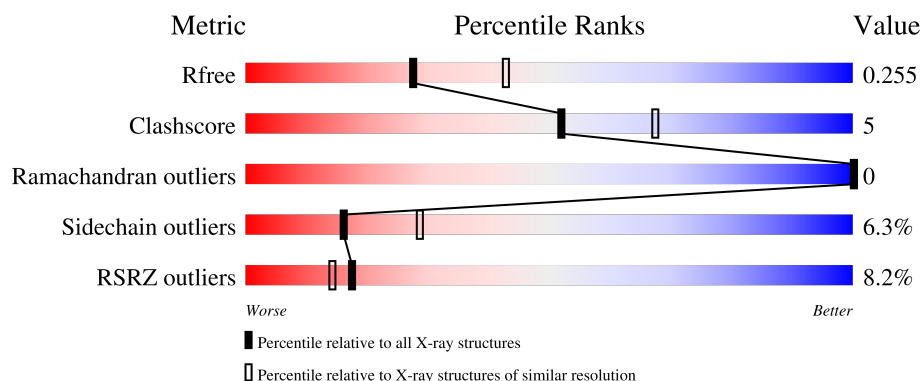
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	628	<div> <div>5%</div> <div>52%</div> <div>9%</div> <div>38%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3273 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 Glutathione S-transferase class-mu 26 kDa isozyme,E3 ubiquitin-protein ligase CBL.

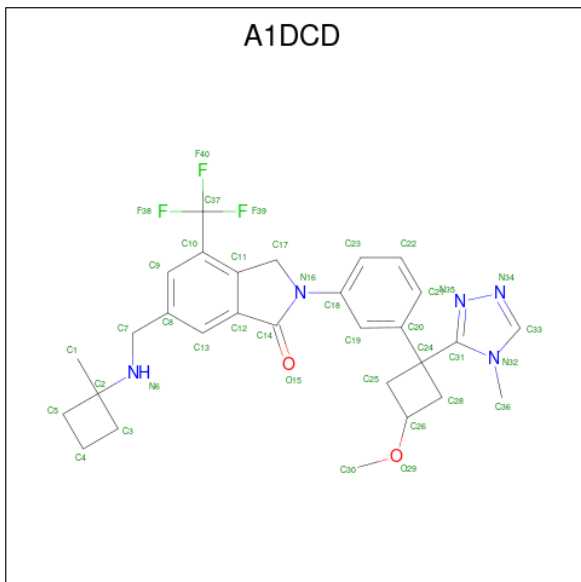
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			3161	2029	530	576	26			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-189	MET	-	initiating methionine	UNP P08515
A	-188	HIS	-	expression tag	UNP P08515
A	-187	HIS	-	expression tag	UNP P08515
A	-186	HIS	-	expression tag	UNP P08515
A	-185	HIS	-	expression tag	UNP P08515
A	-184	HIS	-	expression tag	UNP P08515
A	-183	HIS	-	expression tag	UNP P08515
A	-182	GLY	-	expression tag	UNP P08515
A	-49	LYS	GLU	conflict	UNP P08515
A	36	SER	-	linker	UNP P08515
A	37	ASP	-	linker	UNP P08515
A	38	GLY	-	linker	UNP P08515
A	39	GLU	-	linker	UNP P08515
A	40	ASN	-	linker	UNP P08515
A	41	LEU	-	linker	UNP P08515
A	42	TYR	-	linker	UNP P08515
A	43	PHE	-	linker	UNP P08515
A	44	GLN	-	linker	UNP P08515
A	45	GLY	-	linker	UNP P08515
A	46	SER	-	linker	UNP P08515
A	436	GLY	-	expression tag	UNP P22681
A	437	ASN	-	expression tag	UNP P22681
A	438	SER	-	expression tag	UNP P22681

- Molecule 2 is 2-{3-[(1r,3r)-3-methoxy-1-(4-methyl-4H-1,2,4-triazol-3-yl)cyclobutyl]phenyl}-6-[[1-methylcyclobutyl]amino]methyl}-4-(trifluoromethyl)-2,3-dihydro-1H-isoind

ol-1-one (CCD ID: A1DCD) (formula: $\text{C}_{29}\text{H}_{32}\text{F}_3\text{N}_5\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	29	3	5	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	70	Total O 70 70	0	0

i

- Molecule 1: Glutathione S-transferase class-mu 26 kDa isozyme,E3 ubiquitin-protein ligase CBL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.72Å 49.86Å 83.87Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	30.35 – 2.39 30.35 – 2.39	Depositor EDS
% Data completeness (in resolution range)	68.5 (30.35-2.39) 68.7 (30.35-2.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.198 , 0.256 0.198 , 0.255	Depositor DCC
R_{free} test set	605 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3273	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, A1DCD

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	0.16	0/3246	0.31	0/4387

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3161	0	3128	32	0
2	A	39	0	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	70	0	0	0	0
All	All	3273	0	3128	32	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 5.

All (32) 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:398:HIS:CE1	1:A:419:CYS:HB3	2.34	0.63
1:A:390:ASP:H	1:A:401:CYS:HA	1.65	0.62
1:A:389:LYS:HD3	1:A:399:LEU:HD23	1.84	0.59
1:A:99:LEU:HD22	1:A:106:MET:HE3	1.84	0.58
1:A:299:ARG:HH22	1:A:304:ALA:HB2	1.69	0.58
1:A:390:ASP:HB2	1:A:402:THR:HG23	1.90	0.53
1:A:392:LYS:HE2	1:A:397:GLY:HA2	1.91	0.53
1:A:398:HIS:HE1	1:A:419:CYS:HB3	1.72	0.52
1:A:393:ILE:HG23	1:A:423:ILE:HG23	1.91	0.51
1:A:379:GLN:HA	1:A:431:VAL:HG12	1.93	0.51
1:A:65:LYS:HD3	1:A:130:ILE:HD13	1.93	0.50
1:A:160:HIS:CD2	1:A:230:LEU:HB3	2.49	0.48
1:A:285:ILE:HD12	1:A:308:VAL:HG13	1.96	0.48
1:A:78:LYS:HG2	1:A:80:SER:H	1.79	0.48
1:A:396:CYS:SG	1:A:398:HIS:CG	3.08	0.46
1:A:222:MET:HE1	1:A:382:LYS:HA	1.98	0.46
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.51	0.45
1:A:389:LYS:HB2	1:A:431:VAL:HG21	1.98	0.45
1:A:379:GLN:HE21	1:A:380:LEU:HD13	1.81	0.45
1:A:335:GLY:HA2	1:A:338:LEU:HD21	2.00	0.43
1:A:194:PHE:CD1	1:A:200:VAL:HG11	2.54	0.43
1:A:168:ILE:C	1:A:170:PRO:HD3	2.44	0.42
1:A:379:GLN:HG2	1:A:380:LEU:HD13	2.01	0.42
1:A:56:VAL:HG11	1:A:99:LEU:HD11	2.01	0.42
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.90	0.42
1:A:78:LYS:HE2	1:A:80:SER:HB3	2.01	0.42
1:A:215:ILE:HG21	1:A:221:ALA:HB2	2.02	0.42
1:A:261:LEU:HD13	1:A:324:LEU:HD23	2.01	0.42
1:A:95:LEU:O	1:A:99:LEU:HG	2.20	0.41
1:A:148:ARG:HD2	1:A:148:ARG:HA	1.86	0.41
1:A:98:ILE:HG12	1:A:172:GLY:HA2	2.03	0.41
1:A:285:ILE:HD13	1:A:314:ILE:HG13	2.03	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	389/628 (62%)	378 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	352/561 (63%)	330 (94%)	22 (6%)	16	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	MET
1	A	192	LYS
1	A	196	GLU
1	A	203	LYS
1	A	219	LEU
1	A	299	ARG
1	A	334	GLU
1	A	345	GLN
1	A	361	ILE
1	A	362	LYS
1	A	380	LEU
1	A	391	VAL
1	A	392	LYS
1	A	396	CYS
1	A	416	CYS
1	A	421	CYS
1	A	422	GLU
1	A	424	LYS
1	A	427	GLU
1	A	429	ILE
1	A	430	VAL

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Mol	Chain	Res	Type
1	A	432	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	282	GLN
1	A	345	GLN
1	A	414	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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$
2	A1DCD	A	501	-	41,44,44	7.34	17 (41%)	55,69,69	2.68	14 (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
2	A1DCD	A	501	-	-	5/21/60/60	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1DCD	C9-C8	-24.23	0.98	1.39
2	A	501	A1DCD	C13-C8	-23.25	1.00	1.39
2	A	501	A1DCD	C11-C10	18.30	1.67	1.40
2	A	501	A1DCD	C9-C10	-15.69	1.17	1.39
2	A	501	A1DCD	C12-C11	11.61	1.62	1.39
2	A	501	A1DCD	C17-C11	-11.61	1.37	1.50
2	A	501	A1DCD	O15-C14	8.15	1.39	1.22
2	A	501	A1DCD	C12-C14	-6.28	1.38	1.48
2	A	501	A1DCD	C3-C2	-4.32	1.51	1.55
2	A	501	A1DCD	O29-C26	-3.72	1.34	1.43
2	A	501	A1DCD	C5-C2	-3.57	1.51	1.55
2	A	501	A1DCD	C2-N6	-3.41	1.41	1.47
2	A	501	A1DCD	C14-N16	3.32	1.45	1.38
2	A	501	A1DCD	C18-N16	3.14	1.49	1.43
2	A	501	A1DCD	C31-N32	-3.11	1.33	1.36
2	A	501	A1DCD	C13-C12	3.07	1.44	1.39
2	A	501	A1DCD	C25-C24	-2.18	1.51	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1DCD	C10-C9-C8	13.62	145.40	122.26
2	A	501	A1DCD	C11-C17-N16	5.85	108.69	102.53
2	A	501	A1DCD	C17-C11-C12	-5.77	106.19	109.82
2	A	501	A1DCD	C9-C10-C37	3.91	126.08	116.60
2	A	501	A1DCD	C13-C8-C9	3.22	123.38	119.01
2	A	501	A1DCD	F39-C37-C10	-3.18	107.01	112.65
2	A	501	A1DCD	C13-C12-C11	-3.05	120.42	123.27
2	A	501	A1DCD	C25-C24-C20	2.99	123.61	115.97
2	A	501	A1DCD	C36-N32-C31	-2.73	126.70	129.05
2	A	501	A1DCD	F40-C37-C10	-2.60	108.03	112.65
2	A	501	A1DCD	N32-C31-N35	-2.53	107.91	111.36
2	A	501	A1DCD	C11-C12-C14	-2.42	106.54	108.62
2	A	501	A1DCD	N32-C33-N34	-2.20	109.38	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1DCD	C13-C12-C14	2.13	133.04	129.39

There are no chirality outliers.

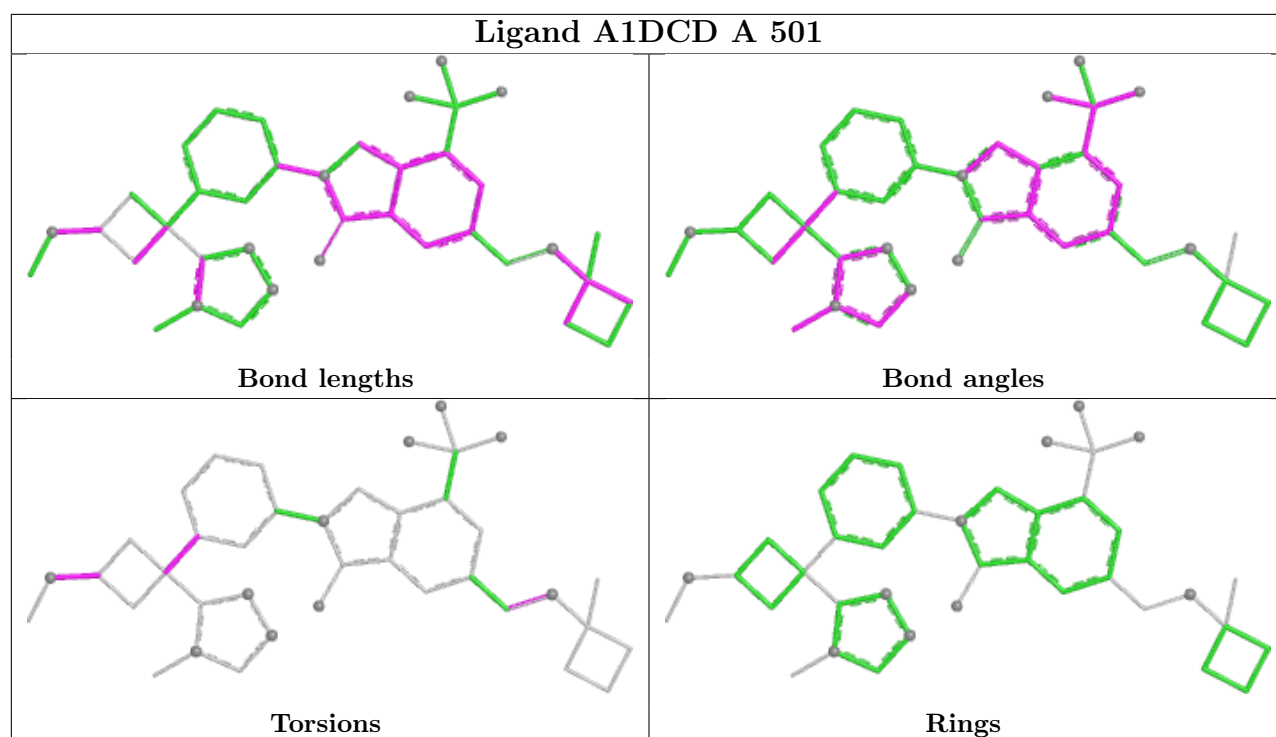
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1DCD	C28-C26-O29-C30
2	A	501	A1DCD	C8-C7-N6-C2
2	A	501	A1DCD	C19-C20-C24-C31
2	A	501	A1DCD	C21-C20-C24-C31
2	A	501	A1DCD	C21-C20-C24-C25

There are no ring outliers.

No monomer is involved in short contacts.

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	389/628 (61%)	0.48	32 (8%) 17 14	26, 53, 151, 236	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	7.9
1	A	380	LEU	3.9
1	A	430	VAL	3.8
1	A	399	LEU	3.8
1	A	434	PHE	3.7
1	A	378	PHE	3.3
1	A	361	ILE	3.0
1	A	395	PRO	3.0
1	A	424	LYS	2.9
1	A	141	TYR	2.9
1	A	432	ASP	2.9
1	A	47	PRO	2.8
1	A	360	HIS	2.7
1	A	433	PRO	2.7
1	A	385	ALA	2.7
1	A	423	ILE	2.7
1	A	379	GLN	2.6
1	A	73	PRO	2.5
1	A	414	GLN	2.5
1	A	435	ASP	2.4
1	A	405	LEU	2.4
1	A	386	GLU	2.4
1	A	421	CYS	2.3
1	A	428	PRO	2.3
1	A	426	THR	2.2
1	A	408	TRP	2.2
1	A	411	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	ILE	2.2
1	A	418	PHE	2.2
1	A	401	CYS	2.1
1	A	417	PRO	2.1
1	A	79	ASN	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](#)

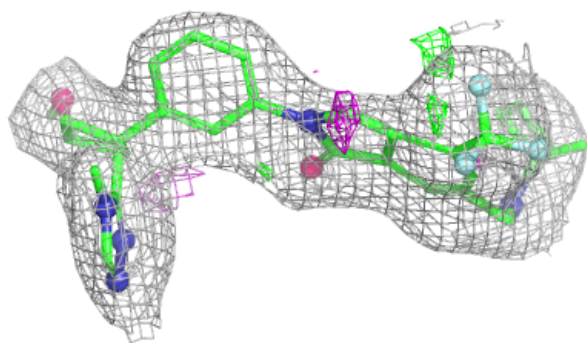
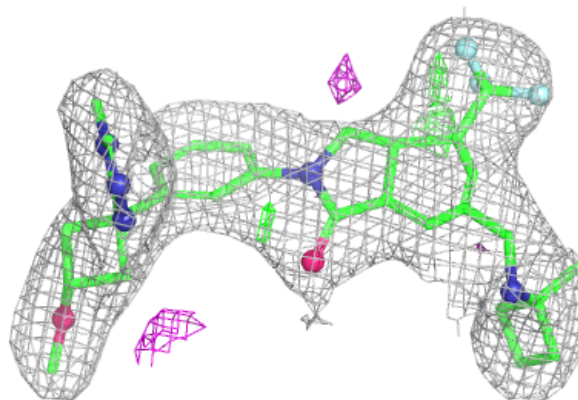
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	502	1/1	0.84	0.08	143,143,143,143	1
2	A1DCD	A	501	39/39	0.91	0.09	28,37,55,75	0
3	ZN	A	503	1/1	0.97	0.06	84,84,84,84	1
4	MG	A	504	1/1	0.97	0.04	49,49,49,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1DCD A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.