



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2025 – 02:09 PM EDT

PDB ID : 9O91 / pdb_00009o91
Title : Structure of IKZF2:CRBN:Compound 5 ternary structure
Authors : Strickland, C.O.; Rice, C.T.
Deposited on : 2025-04-17
Resolution : 1.86 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

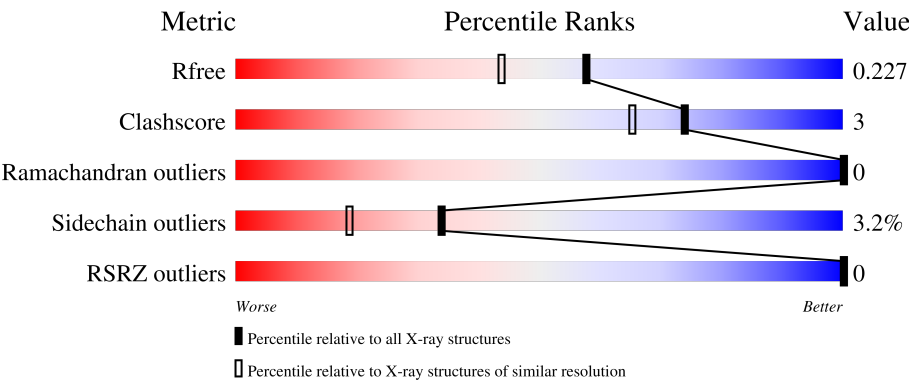
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	111	
1	C	111	
1	E	111	
1	G	111	
2	B	30	

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Mol	Chain	Length	Quality of chain
2	D	30	 83%13%
2	F	30	 87%13%
2	H	30	 80%7%13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4683 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 Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			859	551	142	160	6			
1	C	109	Total	C	N	O	S	0	0	0
			845	543	140	156	6			
1	E	111	Total	C	N	O	S	0	0	0
			862	553	145	158	6			
1	G	109	Total	C	N	O	S	0	0	0
			847	543	142	156	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	GLY	-	expression tag	UNP Q96SW2
A	317	PRO	-	expression tag	UNP Q96SW2
A	318	SER	CYS	engineered mutation	UNP Q96SW2
A	322	SER	CYS	engineered mutation	UNP Q96SW2
A	343	SER	CYS	engineered mutation	UNP Q96SW2
A	366	SER	CYS	engineered mutation	UNP Q96SW2
C	316	GLY	-	expression tag	UNP Q96SW2
C	317	PRO	-	expression tag	UNP Q96SW2
C	318	SER	CYS	engineered mutation	UNP Q96SW2
C	322	SER	CYS	engineered mutation	UNP Q96SW2
C	343	SER	CYS	engineered mutation	UNP Q96SW2
C	366	SER	CYS	engineered mutation	UNP Q96SW2
E	316	GLY	-	expression tag	UNP Q96SW2
E	317	PRO	-	expression tag	UNP Q96SW2
E	318	SER	CYS	engineered mutation	UNP Q96SW2
E	322	SER	CYS	engineered mutation	UNP Q96SW2
E	343	SER	CYS	engineered mutation	UNP Q96SW2
E	366	SER	CYS	engineered mutation	UNP Q96SW2
G	316	GLY	-	expression tag	UNP Q96SW2
G	317	PRO	-	expression tag	UNP Q96SW2
G	318	SER	CYS	engineered mutation	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	322	SER	CYS	engineered mutation	UNP Q96SW2
G	343	SER	CYS	engineered mutation	UNP Q96SW2
G	366	SER	CYS	engineered mutation	UNP Q96SW2

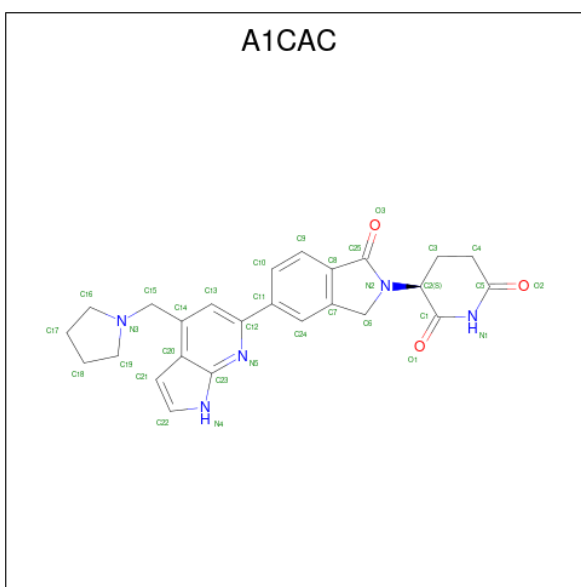
- Molecule 2 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			218	135	45	36	2			
2	D	26	Total	C	N	O	S	0	0	0
			209	130	44	33	2			
2	F	26	Total	C	N	O	S	0	0	0
			209	130	44	33	2			
2	H	26	Total	C	N	O	S	0	0	0
			209	130	44	33	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	135	GLY	-	expression tag	UNP Q9UKS7
D	135	GLY	-	expression tag	UNP Q9UKS7
F	135	GLY	-	expression tag	UNP Q9UKS7
H	135	GLY	-	expression tag	UNP Q9UKS7

- Molecule 3 is (3S)-3-[(5M)-1-oxo-5-{4-[(pyrrolidin-1-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-6-yl}-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: A1CAC) (formula: C₂₅H₂₅N₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 25	N 5	O 3	0	0
3	C	1	Total 33	C 25	N 5	O 3	0	0
3	E	1	Total 33	C 25	N 5	O 3	0	0
3	G	1	Total 33	C 25	N 5	O 3	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total 60	O 60	0	0
5	B	15	Total 15	O 15	0	0
5	C	53	Total 53	O 53	0	0
5	D	13	Total 13	O 13	0	0
5	E	61	Total 61	O 61	0	0
5	F	12	Total 12	O 12	0	0
5	G	56	Total 56	O 56	0	0
5	H	15	Total 15	O 15	0	0

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 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: Protein cereblon

Chain A:  95% 5% .




- Molecule 1: Protein cereblon

Chain C:  87% 9% ..




- Molecule 1: Protein cereblon

Chain E:  90% 9% .



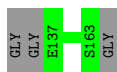
- Molecule 1: Protein cereblon

Chain G:  86% 11% ..




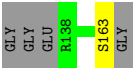
- Molecule 2: Zinc finger protein Helios

Chain B:  90% 10%

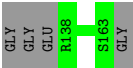
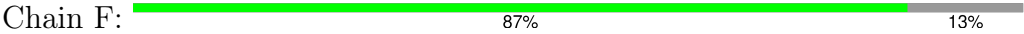


- Molecule 2: Zinc finger protein Helios

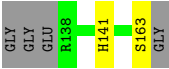
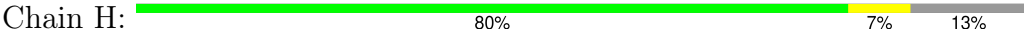
Chain D:  83% 13%



- Molecule 2: Zinc finger protein Helios



- Molecule 2: Zinc finger protein Helios



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.16Å 70.18Å 78.71Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	46.20 – 1.86 46.20 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.20-1.86) 98.4 (46.20-1.86)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.175 , 0.218 0.187 , 0.227	Depositor DCC
R_{free} test set	2032 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4683	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4260e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, A1CAC

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	0.58	0/885	0.94	0/1205
1	C	0.56	0/870	0.95	0/1184
1	E	0.57	0/888	0.97	0/1208
1	G	0.55	0/872	0.97	0/1187
2	B	0.67	0/223	0.98	0/297
2	D	0.67	0/214	1.04	0/285
2	F	0.68	0/214	0.97	0/285
2	H	0.67	0/214	1.05	1/285 (0.4%)
All	All	0.59	0/4380	0.97	1/5936 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	141	HIS	CA-CB-CG	-5.00	108.80	113.80

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	859	0	837	5	0
1	C	845	0	825	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	862	0	846	9	0
1	G	847	0	825	10	0
2	B	218	0	211	0	0
2	D	209	0	205	0	0
2	F	209	0	205	0	0
2	H	209	0	205	0	0
3	A	33	0	0	0	0
3	C	33	0	0	0	0
3	E	33	0	0	0	0
3	G	33	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	60	0	0	1	0
5	B	15	0	0	0	0
5	C	53	0	0	1	0
5	D	13	0	0	0	0
5	E	61	0	0	0	0
5	F	12	0	0	0	0
5	G	56	0	0	0	0
5	H	15	0	0	0	0
All	All	4683	0	4159	26	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 3.

All (26) 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:426:ILE:HD12	5:A:638:HOH:O	1.83	0.79
1:G:406:LYS:O	1:G:409:MET:HG3	1.97	0.64
1:C:319:THR:HB	1:C:334:LYS:HD3	1.81	0.63
1:A:406:LYS:O	1:A:409:MET:HG3	1.99	0.63
1:C:406:LYS:O	1:C:409:MET:HG3	1.99	0.61
1:E:406:LYS:O	1:E:409:MET:HG3	2.00	0.61
1:A:369:ASN:ND2	1:C:369:ASN:ND2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ASN:ND2	1:G:369:ASN:ND2	2.54	0.55
1:E:321:LEU:HD21	1:E:426:ILE:HD11	1.89	0.54
1:G:319:THR:HB	1:G:334:LYS:HD3	1.90	0.53
1:C:329:THR:HG21	1:C:391:CYS:SG	2.51	0.50
1:G:329:THR:HG21	1:G:391:CYS:SG	2.52	0.49
1:G:404:ALA:HB1	1:G:409:MET:HG3	1.95	0.48
1:G:409:MET:HE2	1:G:409:MET:HB3	1.78	0.46
1:E:404:ALA:HB1	1:E:409:MET:HG3	1.96	0.46
1:C:419:ARG:HG3	1:C:426:ILE:HD12	1.98	0.45
1:C:426:ILE:CD1	5:C:636:HOH:O	2.65	0.45
1:E:369:ASN:HD21	1:G:369:ASN:ND2	2.14	0.44
1:E:409:MET:HE2	1:E:409:MET:HB3	1.81	0.43
1:E:320:SER:HB3	1:E:330:GLU:OE2	2.19	0.43
1:A:409:MET:HE2	1:A:409:MET:HB3	1.77	0.42
1:E:369:ASN:ND2	1:G:369:ASN:HD21	2.18	0.42
1:A:369:ASN:HD21	1:C:369:ASN:ND2	2.17	0.41
1:G:424:PRO:O	1:G:426:ILE:HD12	2.21	0.40
1:G:329:THR:HG23	1:G:331:ILE:HD11	2.03	0.40
1:E:371:ILE:HD11	1:E:390:GLN:NE2	2.36	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	109/111 (98%)	108 (99%)	1 (1%)	0	100	100
1	C	107/111 (96%)	106 (99%)	1 (1%)	0	100	100
1	E	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
1	G	107/111 (96%)	104 (97%)	3 (3%)	0	100	100
2	B	25/30 (83%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
2	F	24/30 (80%)	24 (100%)	0	0	100	100
2	H	24/30 (80%)	24 (100%)	0	0	100	100
All	All	529/564 (94%)	519 (98%)	10 (2%)	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	95/96 (99%)	92 (97%)	3 (3%)	34	19
1	C	93/96 (97%)	88 (95%)	5 (5%)	18	6
1	E	95/96 (99%)	93 (98%)	2 (2%)	48	34
1	G	93/96 (97%)	90 (97%)	3 (3%)	34	19
2	B	24/24 (100%)	24 (100%)	0	100	100
2	D	23/24 (96%)	22 (96%)	1 (4%)	25	10
2	F	23/24 (96%)	23 (100%)	0	100	100
2	H	23/24 (96%)	22 (96%)	1 (4%)	25	10
All	All	469/480 (98%)	454 (97%)	15 (3%)	34	19

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	LEU
1	A	351	ASN
1	A	409	MET
1	C	342	LEU
1	C	351	ASN
1	C	390	GLN
1	C	409	MET
1	C	426	ILE

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Mol	Chain	Res	Type
2	D	163	SER
1	E	342	LEU
1	E	409	MET
1	G	351	ASN
1	G	373	ARG
1	G	409	MET
2	H	163	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	A	390	GLN
2	B	143	ASN
1	C	335	ASN
1	C	369	ASN
1	C	378	HIS
1	C	390	GLN
2	D	151	GLN
2	D	154	ASN
1	E	327	GLN
1	E	369	ASN
1	E	390	GLN
2	F	144	GLN
2	F	154	ASN
1	G	369	ASN
1	G	378	HIS
1	G	390	GLN
2	H	141	HIS
2	H	154	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1CAC	A	501	-	36,38,38	0.74	0	48,56,56	0.96	2 (4%)
3	A1CAC	C	501	-	36,38,38	0.69	0	48,56,56	0.87	1 (2%)
3	A1CAC	G	501	-	36,38,38	0.68	0	48,56,56	0.91	2 (4%)
3	A1CAC	E	501	-	36,38,38	0.71	0	48,56,56	0.87	1 (2%)

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
3	A1CAC	A	501	-	-	0/12/44/44	0/6/6/6
3	A1CAC	C	501	-	-	2/12/44/44	0/6/6/6
3	A1CAC	G	501	-	-	2/12/44/44	0/6/6/6
3	A1CAC	E	501	-	-	0/12/44/44	0/6/6/6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	A1CAC	C1-C2-N2	-3.29	107.28	110.32
3	G	501	A1CAC	C1-C2-N2	-2.62	107.90	110.32
3	E	501	A1CAC	C1-C2-N2	-2.49	108.02	110.32
3	A	501	A1CAC	C19-N3-C16	-2.12	101.55	104.04
3	G	501	A1CAC	C11-C24-C7	-2.10	118.80	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	501	A1CAC	C1-C2-N2	-2.06	108.42	110.32

There are no chirality outliers.

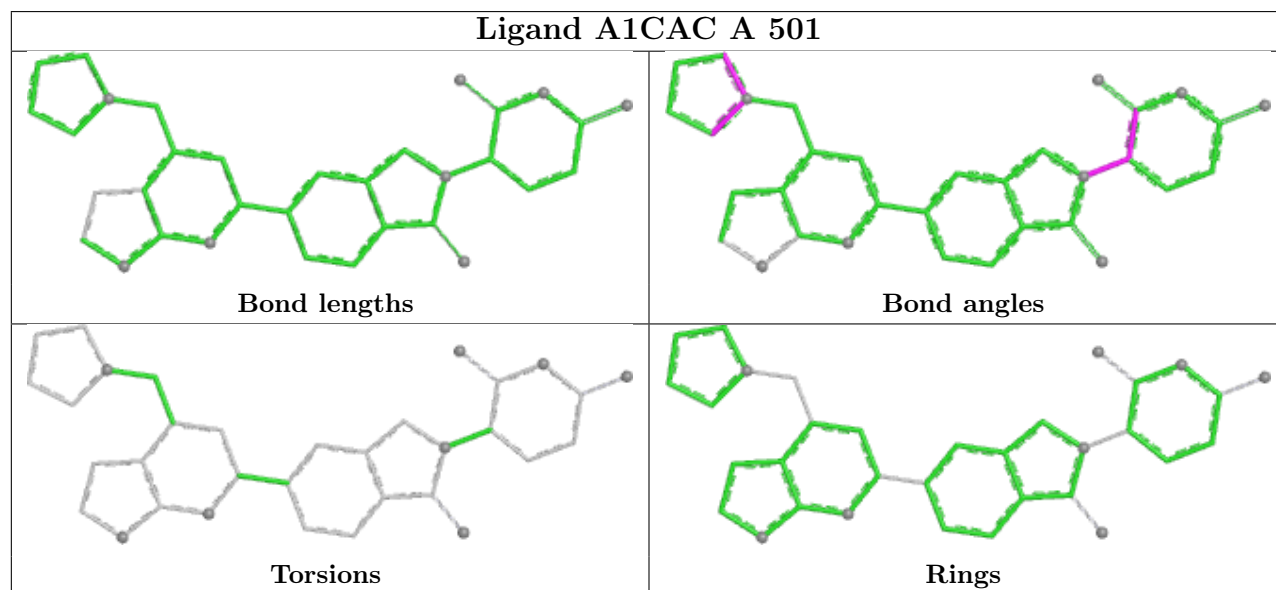
All (4) torsion outliers are listed below:

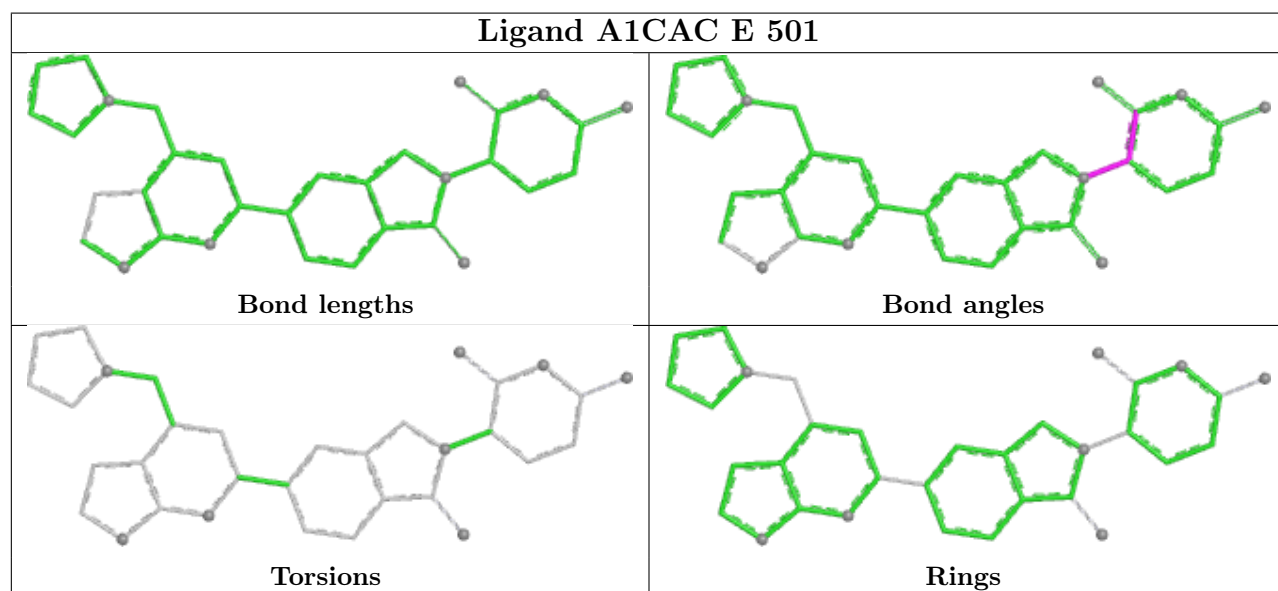
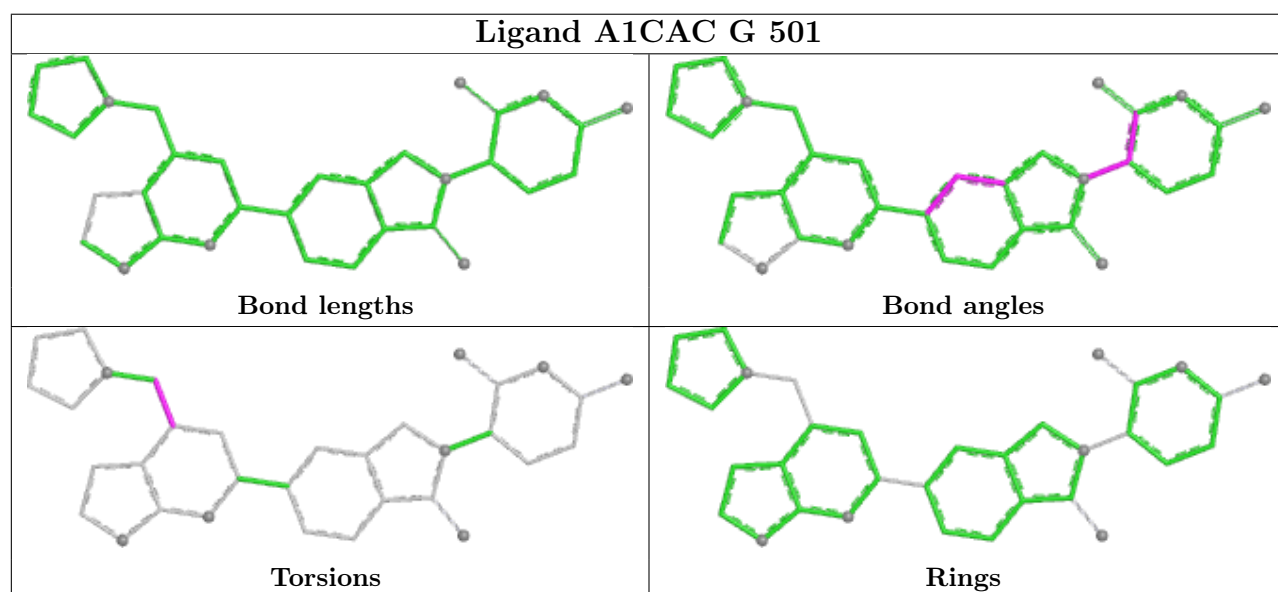
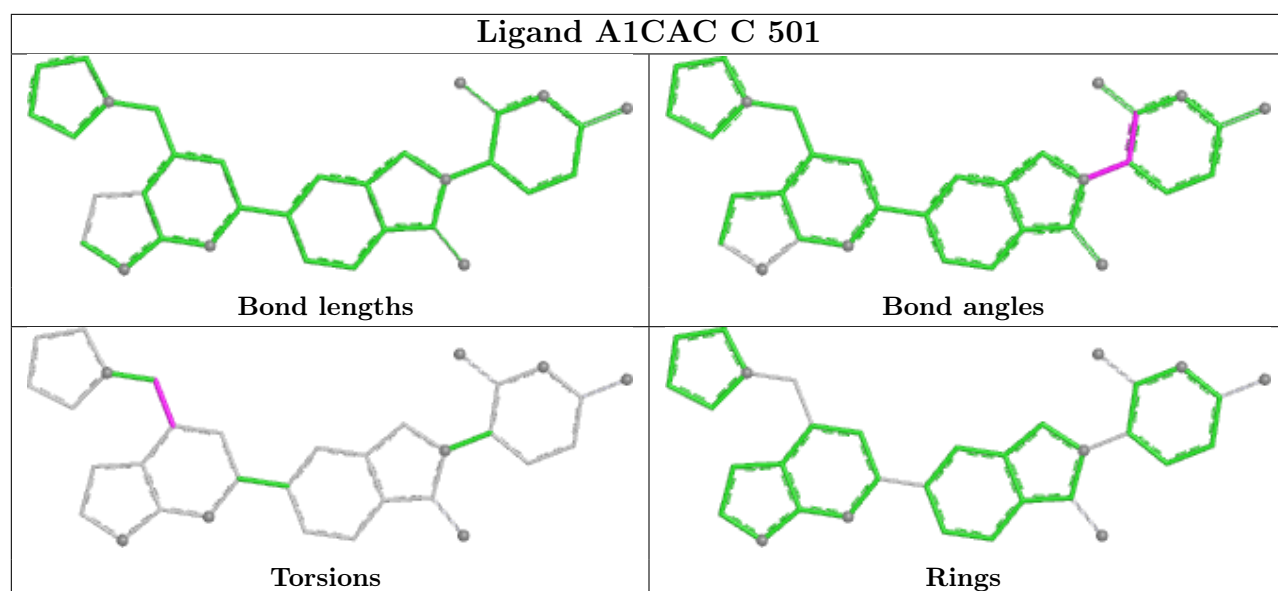
Mol	Chain	Res	Type	Atoms
3	C	501	A1CAC	C13-C14-C15-N3
3	C	501	A1CAC	C20-C14-C15-N3
3	G	501	A1CAC	C20-C14-C15-N3
3	G	501	A1CAC	C13-C14-C15-N3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	111/111 (100%)	-1.47	0 100 100	11, 18, 33, 60	0
1	C	109/111 (98%)	-1.43	0 100 100	12, 18, 38, 52	0
1	E	111/111 (100%)	-1.43	0 100 100	12, 18, 35, 52	0
1	G	109/111 (98%)	-1.41	0 100 100	12, 18, 39, 55	0
2	B	27/30 (90%)	-1.42	0 100 100	14, 18, 35, 53	0
2	D	26/30 (86%)	-1.39	0 100 100	14, 18, 30, 51	0
2	F	26/30 (86%)	-1.41	0 100 100	14, 19, 30, 40	0
2	H	26/30 (86%)	-1.44	0 100 100	14, 18, 29, 51	0
All	All	545/564 (96%)	-1.43	0 100 100	11, 18, 39, 60	0

There are no RSRZ outliers to report.

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](#)

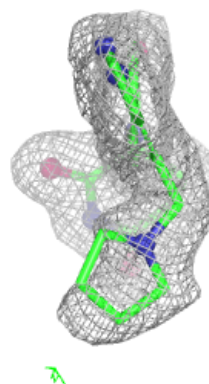
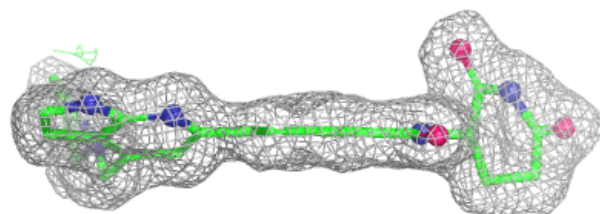
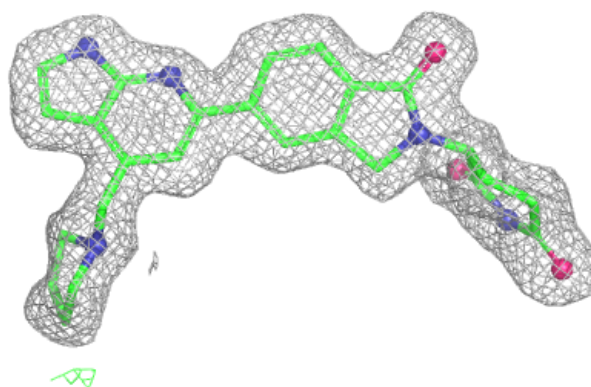
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1CAC	A	501	33/33	0.99	0.03	12,14,36,38	0
3	A1CAC	C	501	33/33	0.99	0.03	11,13,25,26	0
3	A1CAC	E	501	33/33	0.99	0.03	12,15,35,36	0
3	A1CAC	G	501	33/33	0.99	0.03	11,14,25,25	0
4	ZN	A	502	1/1	1.00	0.01	16,16,16,16	0
4	ZN	B	201	1/1	1.00	0.01	15,15,15,15	0
4	ZN	C	502	1/1	1.00	0.01	16,16,16,16	0
4	ZN	D	201	1/1	1.00	0.01	14,14,14,14	0
4	ZN	E	502	1/1	1.00	0.01	16,16,16,16	0
4	ZN	F	201	1/1	1.00	0.01	14,14,14,14	0
4	ZN	G	502	1/1	1.00	0.01	16,16,16,16	0
4	ZN	H	201	1/1	1.00	0.01	14,14,14,14	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.

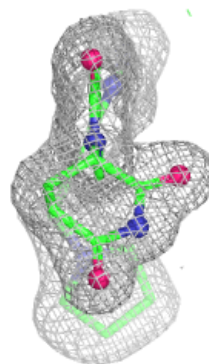
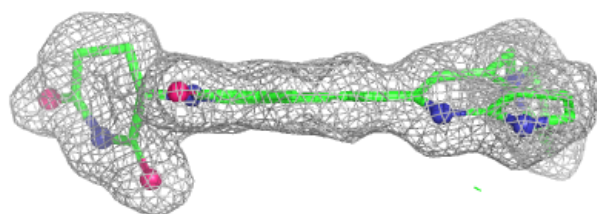
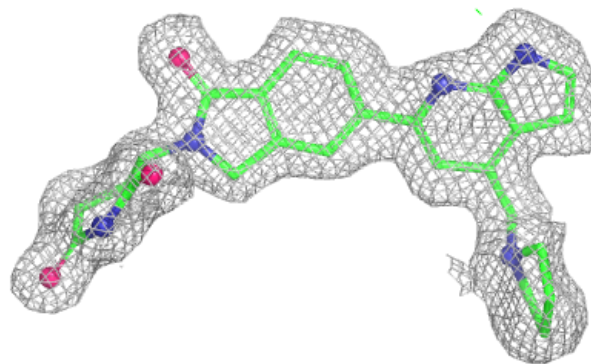
Electron density around A1CAC A 501:

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

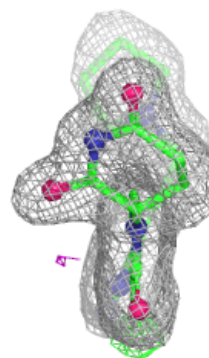
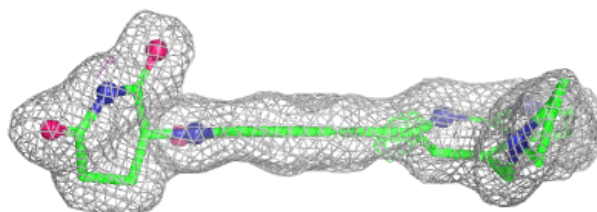
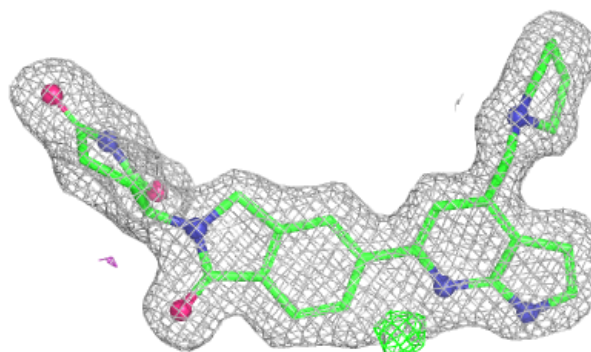


Electron density around A1CAC C 501:

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

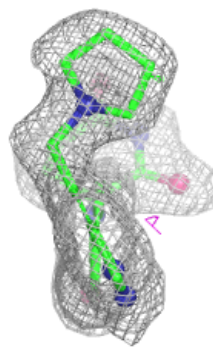
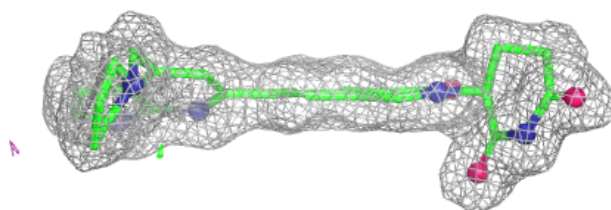
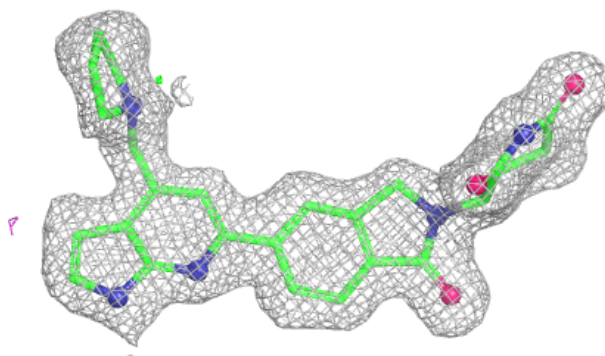
**Electron density around A1CAC E 501:**

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



Electron density around A1CAC G 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 [i](#)

There are no such residues in this entry.