



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 10:57 AM EDT

PDB ID : 9DOM / pdb\_00009dom  
Title : PVTX-405: A Potent, Highly Selective, and Orally Efficacious Molecular Glue  
Degradar of IKZF2 for Cancer Immunotherapy  
Authors : Strickland, C.O.; Rice, C.T.  
Deposited on : 2024-09-19  
Resolution : 1.69 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](mailto: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:

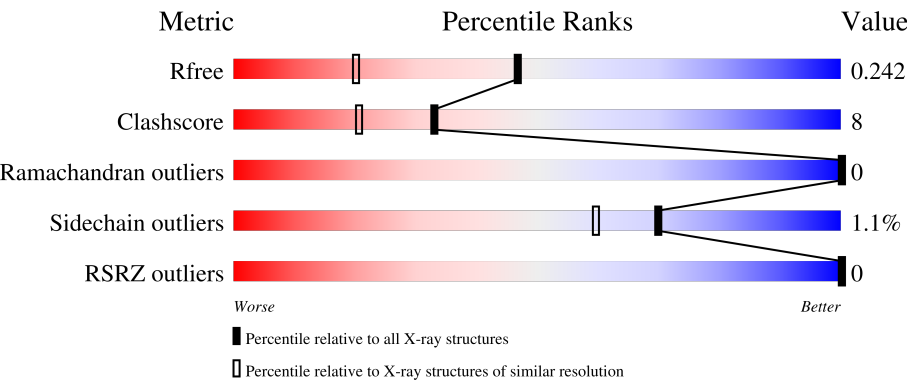
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

# 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 1.69 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 <sub>free</sub>	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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  $\geq 3$ , 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	<div><div>80%</div><div>14%</div><div>.</div><div>.</div></div>
1	C	111	<div><div>76%</div><div>22%</div><div>.</div><div>.</div></div>
1	E	111	<div><div>80%</div><div>17%</div><div>.</div><div>.</div></div>
1	G	111	<div><div>88%</div><div>9%</div><div>.</div></div>
2	B	30	<div><div>80%</div><div>7%</div><div>.</div><div>10%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	30	<div><div></div><div>80%7%13%</div></div>
2	F	30	<div><div></div><div>70%17%13%</div></div>
2	H	30	<div><div></div><div>77%7%13%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4636 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	107	Total	C	N	O	S	0	0	0
			830	534	137	153	6			
1	C	109	Total	C	N	O	S	0	2	0
			853	548	141	158	6			
1	E	109	Total	C	N	O	S	0	0	0
			848	544	140	158	6			
1	G	108	Total	C	N	O	S	0	0	0
			848	544	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	-	expression tag	UNP Q96SW2
A	322	SER	CYS	conflict	UNP Q96SW2
A	343	SER	CYS	conflict	UNP Q96SW2
A	366	SER	CYS	conflict	UNP Q96SW2
C	316	GLY	-	expression tag	UNP Q96SW2
C	317	PRO	-	expression tag	UNP Q96SW2
C	318	SER	-	expression tag	UNP Q96SW2
C	322	SER	CYS	conflict	UNP Q96SW2
C	343	SER	CYS	conflict	UNP Q96SW2
C	366	SER	CYS	conflict	UNP Q96SW2
E	316	GLY	-	expression tag	UNP Q96SW2
E	317	PRO	-	expression tag	UNP Q96SW2
E	318	SER	-	expression tag	UNP Q96SW2
E	322	SER	CYS	conflict	UNP Q96SW2
E	343	SER	CYS	conflict	UNP Q96SW2
E	366	SER	CYS	conflict	UNP Q96SW2
G	316	GLY	-	expression tag	UNP Q96SW2
G	317	PRO	-	expression tag	UNP Q96SW2
G	318	SER	-	expression tag	UNP Q96SW2

*Continued on next page...*

*Continued from previous page...*

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

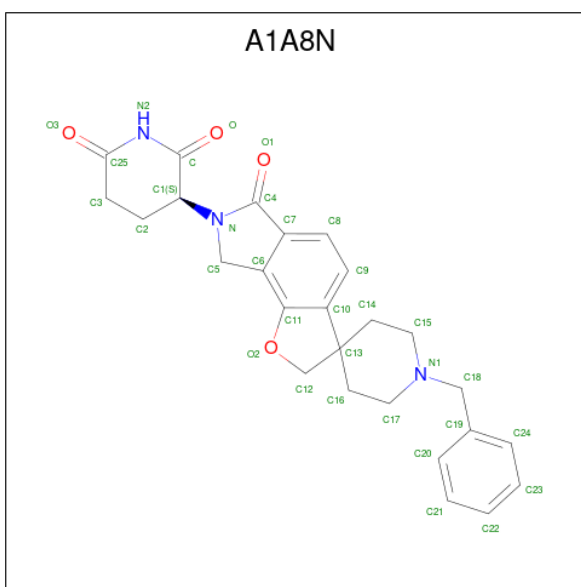
- Molecule 2 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			214	132	44	36	2			
2	D	26	Total	C	N	O	S	0	0	0
			205	128	43	32	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
			212	132	44	34	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-(1'-benzyl-6-oxo-6,8-dihydro-2H,7H-spiro[furo[2,3-e]isoindole-3,4'-piperidin]-7-yl)piperidine-2,6-dione (CCD ID: A1A8N) (formula: C<sub>26</sub>H<sub>27</sub>N<sub>3</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	26	3	4		
3	C	1	Total	C	N	O	0	0
			33	26	3	4		
3	E	1	Total	C	N	O	0	0
			33	26	3	4		
3	G	1	Total	C	N	O	0	0
			33	26	3	4		

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

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


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total 47	O 47	0	0
5	B	20	Total 20	O 20	0	0
5	C	66	Total 66	O 66	0	0
5	D	15	Total 15	O 15	0	0
5	E	57	Total 57	O 57	0	0
5	F	18	Total 18	O 18	0	0
5	G	43	Total 43	O 43	0	0
5	H	11	Total 11	O 11	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: 




- Molecule 1: Protein cereblon

Chain C: 




- Molecule 1: Protein cereblon

Chain E: 




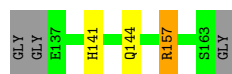
- Molecule 1: Protein cereblon

Chain G: 




- Molecule 2: Zinc finger protein Helios

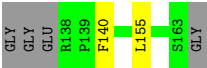
Chain B: 



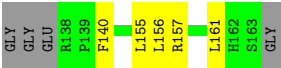
- Molecule 2: Zinc finger protein Helios

Chain D: 





● 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, $\alpha$ , $\beta$ , $\gamma$	45.40Å 69.24Å 79.86Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	79.86 – 1.69 79.86 – 1.69	Depositor EDS
% Data completeness (in resolution range)	84.6 (79.86-1.69) 84.6 (79.86-1.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, $R_{free}$	0.211 , 0.234 0.216 , 0.242	Depositor DCC
$R_{free}$ test set	2166 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 30.84 % 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 1.2235e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, A1A8N

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	0.64	0/854	0.92	1/1161 (0.1%)
1	C	0.66	1/884 (0.1%)	1.06	2/1204 (0.2%)
1	E	0.65	2/873 (0.2%)	0.88	1/1188 (0.1%)
1	G	0.67	2/873 (0.2%)	0.89	0/1187
2	B	0.74	0/219	0.98	0/293
2	D	0.78	0/210	0.91	0/279
2	F	0.72	0/214	0.98	0/285
2	H	0.70	0/217	0.89	0/289
All	All	0.67	5/4344 (0.1%)	0.94	4/5886 (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	1
1	C	0	1
2	B	0	1
2	F	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	378	HIS	CE1-NE2	6.17	1.38	1.32
1	G	378	HIS	CE1-NE2	5.79	1.38	1.32
1	E	357	HIS	CE1-NE2	5.47	1.38	1.32
1	G	353	HIS	CE1-NE2	5.14	1.37	1.32
1	E	378	HIS	CE1-NE2	5.02	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	CYS	CB-CA-C	-17.74	76.61	110.67
1	C	326	CYS	N-CA-C	6.51	119.37	111.82
1	A	326	CYS	CB-CA-C	-5.48	99.69	110.10
1	E	329	THR	CB-CA-C	5.25	119.21	109.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	ARG	Sidechain
2	B	157	ARG	Sidechain
1	C	326	CYS	Mainchain
2	F	157	ARG	Sidechain

## 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	830	0	812	14	0
1	C	853	0	836	24	0
1	E	848	0	827	17	0
1	G	848	0	833	6	0
2	B	214	0	200	7	0
2	D	205	0	197	1	0
2	F	209	0	205	1	0
2	H	212	0	206	2	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	47	0	0	0	0
5	B	20	0	0	2	0
5	C	66	0	0	5	0
5	D	15	0	0	0	0
5	E	57	0	0	3	0
5	F	18	0	0	0	0
5	G	43	0	0	1	0
5	H	11	0	0	1	0
All	All	4636	0	4116	65	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 8.

All (65) 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:E:325:GLN:NE2	5:E:601:HOH:O	1.63	1.28
1:C:398:ILE:HG22	5:C:601:HOH:O	1.49	1.09
1:E:342:LEU:HB2	5:E:651:HOH:O	1.50	1.08
1:C:371:ILE:HD11	1:C:390:GLN:NE2	1.78	0.98
1:C:398:ILE:O	5:C:601:HOH:O	1.92	0.88
1:C:340:LEU:HD23	1:C:381:PHE:CD1	2.09	0.86
1:A:371:ILE:HD11	1:A:390:GLN:OE1	1.76	0.85
1:C:329:THR:OG1	1:C:393:ILE:HD12	1.86	0.76
1:C:324:LYS:HE2	1:C:420:SER:O	1.86	0.76
1:E:324:LYS:HE2	1:E:420:SER:O	1.87	0.75
1:C:398:ILE:C	5:C:601:HOH:O	2.28	0.74
1:C:407:LYS:O	1:E:419:ARG:NH2	2.20	0.73
1:A:318:SER:HB3	1:A:334:LYS:HG3	1.70	0.73
1:E:406:LYS:O	1:E:409:MET:HG3	1.90	0.71
2:B:141:HIS:NE2	5:B:301:HOH:O	2.19	0.68
1:A:319:THR:HG22	1:A:334:LYS:HG2	1.74	0.68
1:C:417:LEU:HA	5:C:601:HOH:O	1.96	0.66
1:C:340:LEU:HD22	1:C:414:PHE:CZ	2.31	0.66
1:C:326:CYS:HB3	1:C:328:GLU:H	1.62	0.65
1:C:360:LEU:HD22	1:C:426:ILE:HD11	1.80	0.63
1:A:318:SER:HB3	1:A:334:LYS:CG	2.31	0.61
1:C:360:LEU:HD22	1:C:426:ILE:CD1	2.32	0.59
1:E:360:LEU:HD22	1:E:426:ILE:HD11	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:LEU:HD13	5:H:304:HOH:O	2.04	0.57
1:A:340:LEU:C	1:A:340:LEU:HD13	2.30	0.56
2:B:157:ARG:NH1	1:E:344:GLY:H	2.05	0.55
1:E:418:THR:HG21	5:E:615:HOH:O	2.05	0.55
1:A:393:ILE:O	1:C:392:LYS:HE3	2.05	0.55
1:C:342:LEU:H	1:C:342:LEU:HD22	1.71	0.55
1:E:340:LEU:C	1:E:340:LEU:HD13	2.31	0.54
1:G:340:LEU:C	1:G:340:LEU:HD13	2.32	0.54
1:G:360:LEU:HD22	1:G:426:ILE:CD1	2.37	0.54
2:B:157:ARG:HH12	1:E:344:GLY:H	1.55	0.53
1:E:340:LEU:HD13	1:E:340:LEU:O	2.09	0.53
1:C:342:LEU:HD22	1:C:342:LEU:N	2.23	0.53
1:C:371:ILE:HD11	1:C:390:GLN:CD	2.34	0.51
1:A:340:LEU:HD13	1:A:340:LEU:O	2.10	0.51
1:C:407:LYS:HD2	5:C:619:HOH:O	2.10	0.50
1:E:324:LYS:CE	1:E:420:SER:O	2.58	0.50
1:G:340:LEU:HD13	1:G:340:LEU:O	2.11	0.50
1:G:369:ASN:ND2	5:G:601:HOH:O	2.45	0.50
1:C:329:THR:HG1	1:C:393:ILE:HD12	1.77	0.48
2:H:140:PHE:HB3	2:H:155:LEU:HD22	1.95	0.48
1:G:423:LEU:HD12	1:G:424:PRO:HA	1.97	0.47
1:A:426:ILE:HG22	1:A:426:ILE:O	2.14	0.46
2:F:140:PHE:HB3	2:F:155:LEU:HD22	1.96	0.46
1:C:324:LYS:CE	1:C:420:SER:O	2.61	0.45
1:C:409:MET:HE3	1:C:409:MET:HB3	1.88	0.45
1:A:371:ILE:HD11	1:A:390:GLN:CD	2.40	0.45
1:C:320:SER:HB3	1:C:330:GLU:HG3	1.98	0.44
2:D:140:PHE:HB3	2:D:155:LEU:HD22	2.00	0.44
1:A:419:ARG:NH1	1:A:426:ILE:OXT	2.45	0.44
2:B:157:ARG:HH11	1:E:344:GLY:HA2	1.83	0.43
1:G:385:ALA:O	1:G:402:PHE:HA	2.19	0.42
1:A:350:VAL:O	1:A:378:HIS:HE1	2.02	0.42
1:E:385:ALA:O	1:E:402:PHE:HA	2.19	0.42
1:A:423:LEU:HA	1:A:424:PRO:C	2.44	0.42
1:A:355:TYR:CZ	2:B:144:GLN:HG2	2.54	0.41
1:C:340:LEU:O	1:C:341:SER:CB	2.67	0.41
2:B:141:HIS:CE1	5:B:301:HOH:O	2.66	0.41
1:A:385:ALA:O	1:A:402:PHE:HA	2.20	0.41
2:B:157:ARG:NH1	1:E:344:GLY:HA2	2.36	0.41
1:C:385:ALA:O	1:C:402:PHE:HA	2.20	0.40
1:E:350:VAL:O	1:E:378:HIS:HE1	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:LEU:HA	1:E:424:PRO:C	2.47	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	103/111 (93%)	101 (98%)	2 (2%)	0	100	100
1	C	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
1	E	107/111 (96%)	105 (98%)	2 (2%)	0	100	100
1	G	106/111 (96%)	104 (98%)	2 (2%)	0	100	100
2	B	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	D	24/30 (80%)	24 (100%)	0	0	100	100
2	F	24/30 (80%)	22 (92%)	2 (8%)	0	100	100
2	H	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	522/564 (93%)	508 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	92/96 (96%)	90 (98%)	2 (2%)	47	30
1	C	95/96 (99%)	95 (100%)	0	100	100
1	E	94/96 (98%)	94 (100%)	0	100	100
1	G	94/96 (98%)	94 (100%)	0	100	100
2	B	23/24 (96%)	23 (100%)	0	100	100
2	D	22/24 (92%)	22 (100%)	0	100	100
2	F	23/24 (96%)	21 (91%)	2 (9%)	8	2
2	H	23/24 (96%)	22 (96%)	1 (4%)	25	10
All	All	466/480 (97%)	461 (99%)	5 (1%)	70	60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	334	LYS
2	F	156	LEU
2	F	161	LEU
2	H	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	GLN
1	A	378	HIS
2	B	144	GLN
2	B	154	ASN
1	C	390	GLN
1	E	378	HIS
2	F	143	ASN
1	G	357	HIS
1	G	369	ASN
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 [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 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	A1A8N	E	501	-	37,38,38	2.03	8 (21%)	52,57,57	3.48	15 (28%)
3	A1A8N	G	501	-	37,38,38	1.82	6 (16%)	52,57,57	3.84	14 (26%)
3	A1A8N	A	501	-	37,38,38	1.72	5 (13%)	52,57,57	3.30	17 (32%)
3	A1A8N	C	501	-	37,38,38	1.91	9 (24%)	52,57,57	4.49	19 (36%)

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	A1A8N	E	501	-	-	0/8/57/57	0/6/6/6
3	A1A8N	G	501	-	-	0/8/57/57	0/6/6/6
3	A1A8N	A	501	-	-	0/8/57/57	0/6/6/6
3	A1A8N	C	501	-	-	0/8/57/57	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	A1A8N	O1-C4	6.24	1.35	1.22
3	E	501	A1A8N	O1-C4	6.20	1.35	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	501	A1A8N	O1-C4	5.38	1.33	1.22
3	G	501	A1A8N	C11-C6	5.01	1.47	1.39
3	E	501	A1A8N	C11-C10	4.40	1.47	1.39
3	A	501	A1A8N	C11-C6	4.28	1.46	1.39
3	A	501	A1A8N	O1-C4	4.16	1.30	1.22
3	A	501	A1A8N	C7-C6	4.16	1.47	1.39
3	A	501	A1A8N	C11-C10	4.15	1.46	1.39
3	E	501	A1A8N	C7-C6	4.00	1.47	1.39
3	E	501	A1A8N	C4-N	-3.82	1.32	1.36
3	E	501	A1A8N	C11-C6	3.80	1.45	1.39
3	C	501	A1A8N	C7-C6	3.45	1.46	1.39
3	G	501	A1A8N	C11-C10	3.43	1.45	1.39
3	C	501	A1A8N	C5-C6	-3.41	1.46	1.50
3	E	501	A1A8N	C5-N	3.41	1.50	1.47
3	E	501	A1A8N	C5-C6	-3.36	1.46	1.50
3	C	501	A1A8N	O2-C11	-3.36	1.33	1.38
3	C	501	A1A8N	C11-C6	3.33	1.44	1.39
3	C	501	A1A8N	C9-C10	-3.04	1.35	1.39
3	A	501	A1A8N	C5-C6	-2.98	1.47	1.50
3	G	501	A1A8N	C7-C6	2.90	1.44	1.39
3	C	501	A1A8N	C4-N	-2.86	1.33	1.36
3	G	501	A1A8N	O2-C11	-2.75	1.34	1.38
3	G	501	A1A8N	C5-C6	-2.54	1.47	1.50
3	C	501	A1A8N	C5-N	2.06	1.49	1.47
3	C	501	A1A8N	C25-N2	-2.04	1.34	1.37
3	E	501	A1A8N	C13-C10	-2.02	1.50	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	A1A8N	C6-C5-N	-21.20	95.38	101.79
3	G	501	A1A8N	C6-C5-N	-17.54	96.49	101.79
3	E	501	A1A8N	C6-C5-N	-14.46	97.42	101.79
3	C	501	A1A8N	C5-C6-C7	12.93	117.94	109.82
3	G	501	A1A8N	C5-C6-C7	11.17	116.83	109.82
3	A	501	A1A8N	C6-C5-N	-10.93	98.48	101.79
3	C	501	A1A8N	C6-C7-C4	-10.44	99.62	108.62
3	A	501	A1A8N	C6-C7-C4	-10.32	99.72	108.62
3	G	501	A1A8N	C6-C7-C4	-9.45	100.47	108.62
3	A	501	A1A8N	C5-C6-C7	9.38	115.71	109.82
3	E	501	A1A8N	C5-N-C1	-9.26	114.86	123.68
3	A	501	A1A8N	C7-C4-N	8.89	112.08	106.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	A1A8N	C5-C6-C7	8.08	114.89	109.82
3	E	501	A1A8N	C6-C7-C4	-7.69	101.99	108.62
3	G	501	A1A8N	C5-N-C1	-7.50	116.54	123.68
3	C	501	A1A8N	C5-N-C4	7.15	116.16	113.15
3	C	501	A1A8N	C5-N-C1	-6.57	117.42	123.68
3	G	501	A1A8N	C7-C4-N	6.53	110.57	106.42
3	C	501	A1A8N	C7-C4-N	6.22	110.38	106.42
3	E	501	A1A8N	C7-C4-N	5.99	110.23	106.42
3	G	501	A1A8N	C5-N-C4	5.54	115.48	113.15
3	A	501	A1A8N	C5-N-C1	-5.50	118.45	123.68
3	C	501	A1A8N	C12-C13-C10	5.41	102.89	99.56
3	E	501	A1A8N	C5-N-C4	5.37	115.41	113.15
3	E	501	A1A8N	C1-N-C4	4.93	129.38	121.86
3	A	501	A1A8N	C15-C14-C13	-4.52	108.63	112.79
3	C	501	A1A8N	C12-O2-C11	4.44	110.67	106.17
3	E	501	A1A8N	O2-C12-C13	4.36	110.56	107.25
3	C	501	A1A8N	C8-C7-C4	4.22	136.67	129.59
3	G	501	A1A8N	C15-C14-C13	-4.03	109.07	112.79
3	G	501	A1A8N	C7-C6-C11	-3.94	112.54	118.81
3	G	501	A1A8N	C1-N-C4	3.82	127.70	121.86
3	E	501	A1A8N	C2-C1-N	-3.63	110.05	114.03
3	G	501	A1A8N	C1-C-N2	3.58	121.47	116.24
3	A	501	A1A8N	C1-N-C4	3.58	127.33	121.86
3	A	501	A1A8N	O1-C4-C7	-3.51	121.86	128.66
3	E	501	A1A8N	C16-C17-N1	3.42	114.65	111.16
3	C	501	A1A8N	C1-C-N2	3.38	121.18	116.24
3	C	501	A1A8N	C7-C6-C11	-3.37	113.44	118.81
3	A	501	A1A8N	C8-C7-C4	3.28	135.09	129.59
3	C	501	A1A8N	C14-C15-N1	3.13	114.35	111.16
3	C	501	A1A8N	C3-C25-N2	3.04	119.93	116.69
3	E	501	A1A8N	C15-C14-C13	-3.00	110.03	112.79
3	E	501	A1A8N	C7-C6-C11	-2.98	114.07	118.81
3	G	501	A1A8N	C8-C7-C4	2.96	134.55	129.59
3	C	501	A1A8N	O1-C4-N	-2.95	123.00	125.34
3	C	501	A1A8N	C15-C14-C13	-2.92	110.10	112.79
3	A	501	A1A8N	O2-C11-C6	2.92	131.19	126.74
3	C	501	A1A8N	C16-C13-C10	-2.91	105.55	111.84
3	A	501	A1A8N	C12-C13-C10	2.85	101.31	99.56
3	A	501	A1A8N	C2-C1-N	-2.76	111.02	114.03
3	E	501	A1A8N	C8-C7-C4	2.73	134.17	129.59
3	C	501	A1A8N	O2-C12-C13	-2.67	105.22	107.25
3	C	501	A1A8N	C1-N-C4	2.64	125.89	121.86

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	A1A8N	C2-C1-N	-2.62	111.17	114.03
3	G	501	A1A8N	O1-C4-C7	-2.56	123.69	128.66
3	A	501	A1A8N	C7-C6-C11	-2.53	114.78	118.81
3	A	501	A1A8N	C1-C-N2	2.50	119.89	116.24
3	E	501	A1A8N	C25-N2-C	-2.49	123.40	126.69
3	G	501	A1A8N	C2-C1-N	-2.48	111.32	114.03
3	A	501	A1A8N	C25-N2-C	-2.35	123.59	126.69
3	E	501	A1A8N	C1-C-N2	2.20	119.45	116.24
3	A	501	A1A8N	C19-C18-N1	-2.18	108.68	113.15
3	G	501	A1A8N	C12-O2-C11	2.09	108.29	106.17
3	A	501	A1A8N	C10-C11-C6	-2.00	118.34	121.65

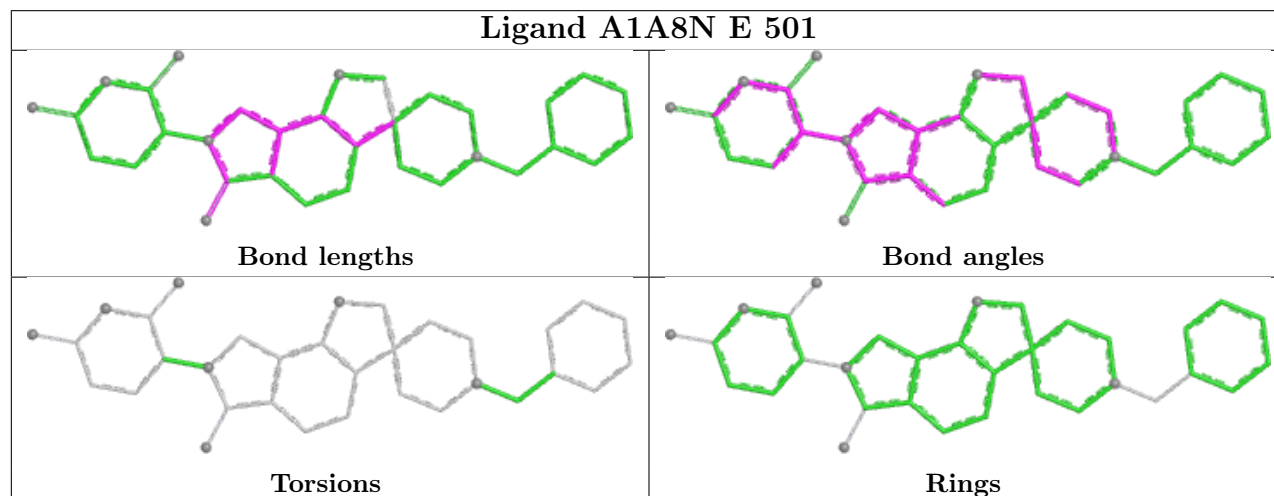
There are no chirality outliers.

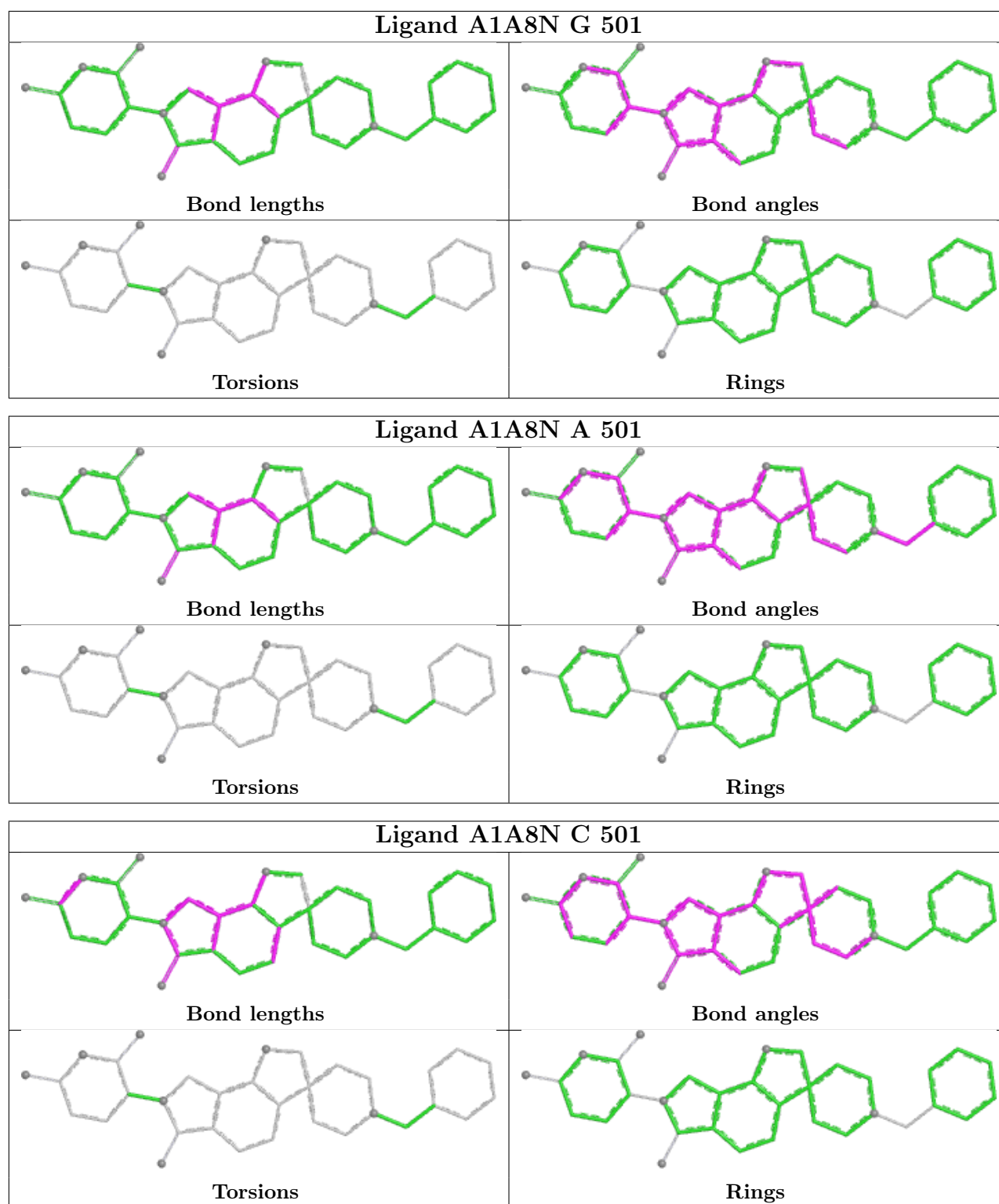
There are no torsion outliers.

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 ⓘ

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	107/111 (96%)	-1.09	0 100 100	17, 24, 42, 71	0
1	C	109/111 (98%)	-1.12	0 100 100	14, 20, 37, 45	2 (1%)
1	E	109/111 (98%)	-1.12	0 100 100	16, 23, 37, 51	0
1	G	108/111 (97%)	-1.14	0 100 100	16, 21, 38, 58	0
2	B	27/30 (90%)	-1.12	0 100 100	18, 24, 37, 45	0
2	D	26/30 (86%)	-1.11	0 100 100	16, 23, 35, 42	0
2	F	26/30 (86%)	-1.13	0 100 100	17, 22, 33, 39	0
2	H	26/30 (86%)	-1.07	0 100 100	19, 25, 35, 45	0
All	All	538/564 (95%)	-1.12	0 100 100	14, 23, 39, 71	2 (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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

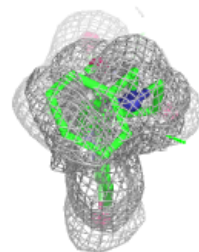
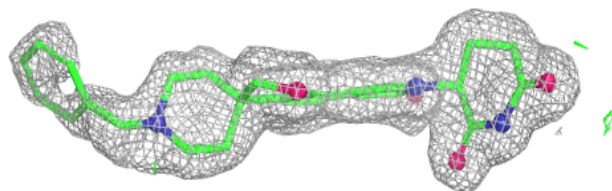
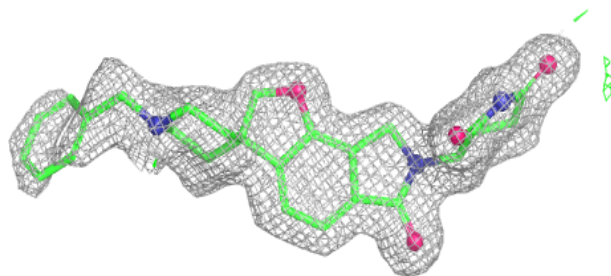
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1A8N	A	501	33/33	0.99	0.03	16,20,41,43	0
3	A1A8N	C	501	33/33	0.99	0.03	15,17,28,29	0
3	A1A8N	E	501	33/33	0.99	0.03	15,18,34,37	0
3	A1A8N	G	501	33/33	0.99	0.04	17,22,41,44	0
4	ZN	A	502	1/1	1.00	0.01	23,23,23,23	0
4	ZN	B	201	1/1	1.00	0.01	19,19,19,19	0
4	ZN	C	502	1/1	1.00	0.01	19,19,19,19	0
4	ZN	D	201	1/1	1.00	0.01	18,18,18,18	0
4	ZN	E	502	1/1	1.00	0.01	22,22,22,22	0
4	ZN	F	201	1/1	1.00	0.01	18,18,18,18	0
4	ZN	G	502	1/1	1.00	0.01	19,19,19,19	0
4	ZN	H	201	1/1	1.00	0.01	20,20,20,20	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 A1A8N A 501:**

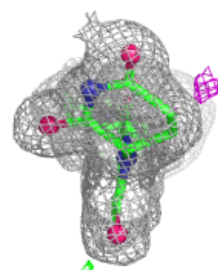
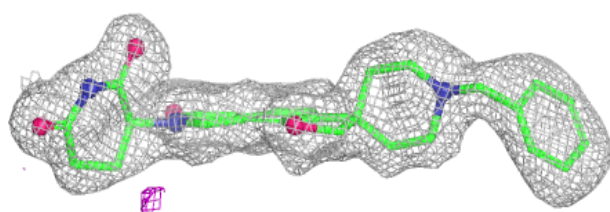
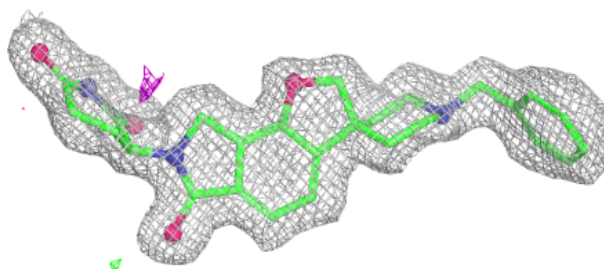
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)



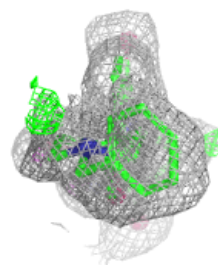
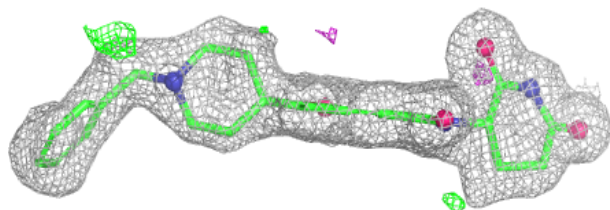
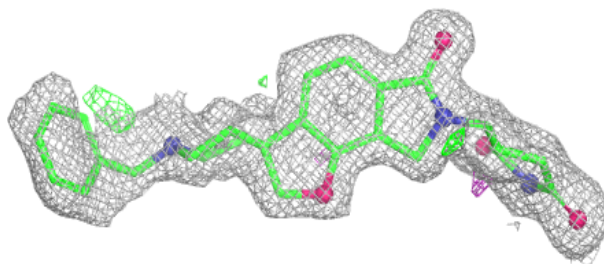


**Electron density around A1A8N C 501:**

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

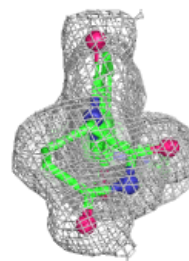
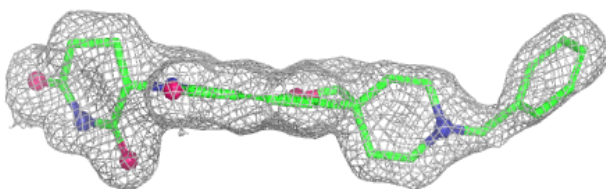
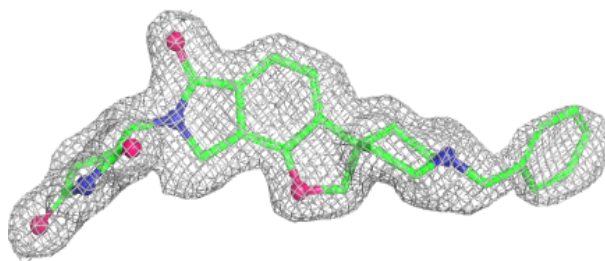
**Electron density around A1A8N E 501:**

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



**Electron density around A1A8N 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.