



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 12:13 PM EDT

PDB ID : 9OHR / pdb\_00009ohr  
Title : Structure of CRBN:IKZF2:Compound 35  
Authors : Strickland, C.O.; Rice, C.T.  
Deposited on : 2025-05-05  
Resolution : 2.34 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) : 2.45.1

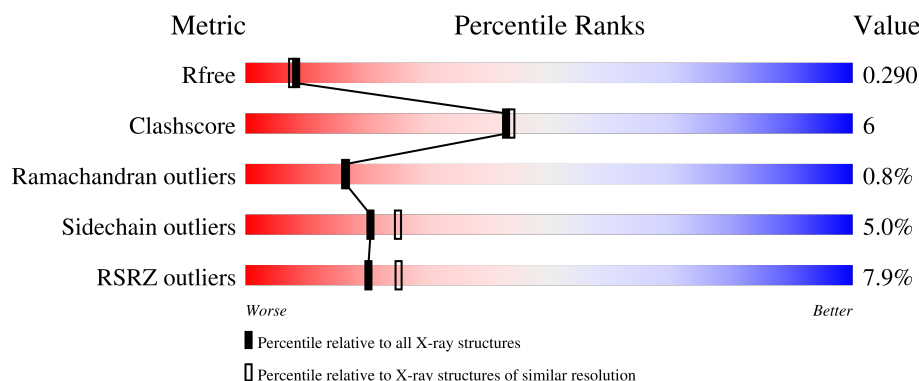
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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>5%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	C	111	<div> <div>7%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	E	111	<div> <div>10%</div> <div>76%</div> <div>19%</div> <div>5%</div> <div>.</div> </div>
1	G	111	<div> <div>8%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	B	30	<div> <div>13%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	30	<div><div><div></div><div></div><div></div></div><div>3%73%13%13%</div></div>
2	F	30	<div><div><div></div><div></div><div></div></div><div>7%73%17%10%</div></div>
2	H	30	<div><div><div></div><div></div><div></div></div><div>7%80%7%10%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4405 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	110	Total	C	N	O	S	0	0	0
			850	544	141	159	6			
1	C	110	Total	C	N	O	S	0	0	0
			853	547	141	159	6			
1	E	110	Total	C	N	O	S	0	0	0
			853	547	141	159	6			
1	G	110	Total	C	N	O	S	0	0	0
			850	544	141	159	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

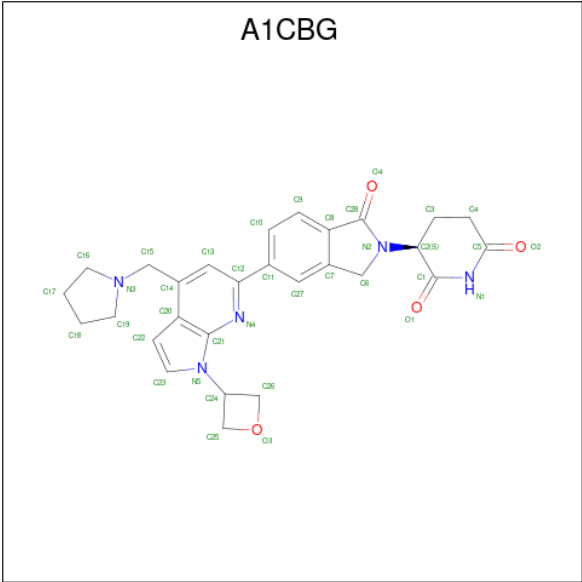
- Molecule 2 is a protein called Zinc finger protein Helios.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	S	0	0	0
			186	117	35	32	2			
2	D	26	Total	C	N	O	S	0	0	0
			195	122	39	32	2			
2	F	27	Total	C	N	O	S	0	0	0
			212	132	42	36	2			
2	H	27	Total	C	N	O	S	0	0	0
			212	132	42	36	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)-5-{1-(oxetan-3-yl)-4-[(pyrrolidin-1-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-6-yl}-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: A1CBG) (formula: C<sub>28</sub>H<sub>29</sub>N<sub>5</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
			37	28	5	4		
3	C	1	Total	C	N	O	0	0
			37	28	5	4		
3	E	1	Total	C	N	O	0	0
			37	28	5	4		
3	G	1	Total	C	N	O	0	0
			37	28	5	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	2	Total	Zn	0	0
			2	2		
4	H	1	Total	Zn	0	0
			1	1		

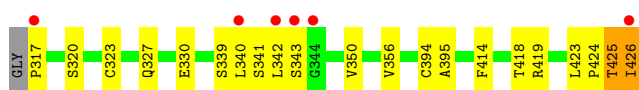
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	3	Total 3	O 3	0	0
5	C	5	Total 5	O 5	0	0
5	D	2	Total 2	O 2	0	0
5	E	9	Total 9	O 9	0	0
5	F	1	Total 1	O 1	0	0
5	G	8	Total 8	O 8	0	0
5	H	2	Total 2	O 2	0	0

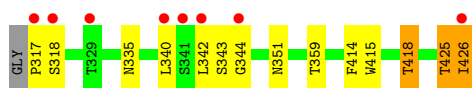
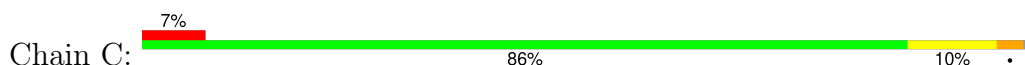
### 3 Residue-property plots [i](#)

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.

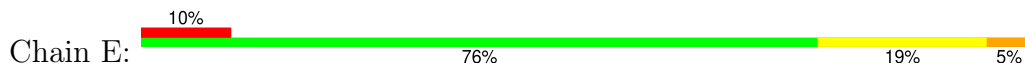
- Molecule 1: Protein cereblon



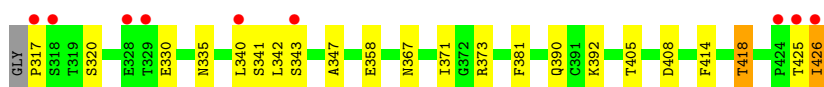
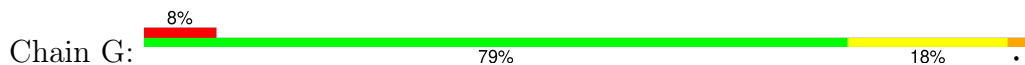
- Molecule 1: Protein cereblon



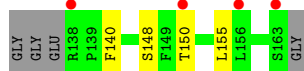
- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon

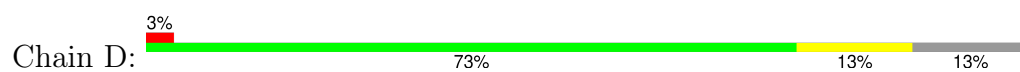


- Molecule 2: Zinc finger protein Helios

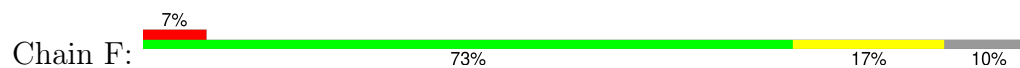


- Molecule 2: Zinc finger protein Helios

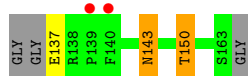
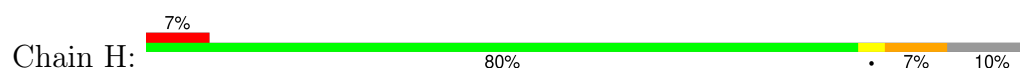




- Molecule 2: Zinc finger protein Helios



- Molecule 2: Zinc finger protein Helios



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.46Å 45.27Å 65.49Å 99.92° 90.58° 104.38°	Depositor
Resolution (Å)	29.68 – 2.34 29.68 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.68-2.34) 94.7 (29.68-2.34)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.224 , 0.290 0.230 , 0.290	Depositor DCC
$R_{free}$ test set	992 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: A1CBG, ZN

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	0.60	0/875	1.06	1/1191 (0.1%)
1	C	0.61	0/878	1.12	4/1195 (0.3%)
1	E	0.60	0/878	1.14	3/1195 (0.3%)
1	G	0.58	0/875	1.11	4/1191 (0.3%)
2	B	0.57	0/191	1.26	1/259 (0.4%)
2	D	0.60	0/200	1.18	0/269
2	F	0.61	0/217	1.08	0/290
2	H	0.57	0/217	1.17	1/290 (0.3%)
All	All	0.60	0/4331	1.12	14/5880 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	150	THR	CA-CB-OG1	-7.05	99.02	109.60
1	G	418	THR	CA-CB-OG1	-6.70	99.55	109.60
1	C	317	PRO	N-CA-CB	6.41	110.05	103.00
1	G	405	THR	CA-CB-OG1	-6.11	100.44	109.60
1	E	317	PRO	N-CA-CB	6.08	109.69	103.00
1	G	317	PRO	N-CA-CB	5.93	109.53	103.00
1	E	418	THR	CA-CB-OG1	-5.87	100.79	109.60
1	A	317	PRO	N-CA-CB	5.84	109.42	103.00
2	H	150	THR	CA-CB-OG1	-5.53	101.30	109.60
1	C	425	THR	CA-CB-OG1	-5.44	101.43	109.60
1	E	329	THR	CA-CB-OG1	-5.39	101.51	109.60
1	C	359	THR	CA-CB-OG1	-5.30	101.65	109.60
1	G	373	ARG	CB-CA-C	5.24	117.13	109.48
1	C	418	THR	CA-CB-OG1	-5.01	102.08	109.60

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	850	0	820	14	0
1	C	853	0	829	7	0
1	E	853	0	829	19	0
1	G	850	0	820	9	0
2	B	186	0	157	2	0
2	D	195	0	177	1	0
2	F	212	0	200	2	0
2	H	212	0	200	2	0
3	A	37	0	0	0	0
3	C	37	0	0	0	0
3	E	37	0	0	0	0
3	G	37	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	2	0	0	0	0
4	H	1	0	0	0	0
5	A	7	0	0	1	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
5	D	2	0	0	0	0
5	E	9	0	0	1	0
5	F	1	0	0	0	0
5	G	8	0	0	1	0
5	H	2	0	0	1	0
All	All	4405	0	4032	51	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 6.

All (51) 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:329:THR:HG21	5:E:603:HOH:O	1.79	0.83
1:A:320:SER:HB3	1:A:330:GLU:OE2	1.83	0.78
1:E:325:GLN:HE21	1:E:325:GLN:HA	1.54	0.72
1:E:341:SER:C	1:E:343:SER:H	2.03	0.66
1:E:374:PRO:HB2	2:H:137:GLU:HG3	1.80	0.63
1:C:342:LEU:C	1:C:344:GLY:H	2.09	0.60
1:G:341:SER:C	1:G:343:SER:H	2.09	0.60
1:A:341:SER:C	1:A:343:SER:H	2.12	0.57
1:E:426:ILE:H	1:E:426:ILE:HD12	1.70	0.57
1:G:340:LEU:HD22	1:G:414:PHE:CZ	2.41	0.56
1:E:340:LEU:HD23	1:E:381:PHE:CD1	2.41	0.55
1:E:341:SER:C	1:E:343:SER:N	2.64	0.54
1:G:320:SER:HB2	1:G:330:GLU:HG3	1.90	0.54
1:G:426:ILE:HD12	5:G:601:HOH:O	2.09	0.53
1:A:423:LEU:HA	1:A:424:PRO:C	2.32	0.53
1:C:340:LEU:HD22	1:C:414:PHE:CZ	2.43	0.53
1:E:320:SER:HB2	1:E:330:GLU:HG3	1.92	0.52
1:G:347:ALA:O	1:G:358:GLU:HA	2.10	0.51
2:H:143:ASN:ND2	5:H:301:HOH:O	2.43	0.50
1:G:341:SER:C	1:G:343:SER:N	2.68	0.50
1:C:426:ILE:HD12	1:C:426:ILE:H	1.76	0.50
1:E:341:SER:O	1:E:343:SER:N	2.45	0.50
1:E:355:TYR:CE2	2:F:144:GLN:HG2	2.47	0.49
1:G:340:LEU:HD23	1:G:381:PHE:CD1	2.49	0.47
1:A:341:SER:C	1:A:343:SER:N	2.72	0.47
1:E:342:LEU:C	1:E:344:GLY:H	2.21	0.47
1:A:426:ILE:H	1:A:426:ILE:HD12	1.79	0.47
1:G:367:ASN:HA	1:G:392:LYS:HD3	1.96	0.47
1:C:318:SER:HA	1:C:335:ASN:OD1	2.15	0.47
1:A:323:CYS:O	1:A:327:GLN:N	2.47	0.47
1:A:419:ARG:NH1	1:E:407:LYS:O	2.48	0.46
1:E:423:LEU:HA	1:E:424:PRO:C	2.39	0.46
1:A:350:VAL:HG22	1:A:356:VAL:HG22	1.97	0.46
1:C:342:LEU:C	1:C:344:GLY:N	2.74	0.46
2:F:140:PHE:HB3	2:F:155:LEU:HD22	1.97	0.45
1:E:374:PRO:HA	1:E:386:TRP:O	2.16	0.45
1:G:371:ILE:HD11	1:G:390:GLN:NE2	2.32	0.45
2:B:140:PHE:HB3	2:B:155:LEU:HD22	2.00	0.44
1:A:394:CYS:O	1:A:395:ALA:HB3	2.18	0.44
1:A:320:SER:CB	1:A:330:GLU:OE2	2.59	0.43
1:E:340:LEU:HD22	1:E:414:PHE:CZ	2.53	0.43
1:A:340:LEU:HD22	1:A:414:PHE:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ILE:HD12	1:C:426:ILE:N	2.33	0.42
1:C:415:TRP:CD1	1:C:415:TRP:N	2.88	0.42
2:D:140:PHE:O	2:D:148:SER:HA	2.20	0.42
1:E:385:ALA:O	1:E:402:PHE:HA	2.20	0.42
1:A:343:SER:O	1:E:413:LYS:CE	2.67	0.41
2:B:140:PHE:O	2:B:148:SER:HA	2.19	0.41
1:A:343:SER:O	1:E:413:LYS:NZ	2.52	0.41
1:A:425:THR:HG23	5:A:604:HOH:O	2.20	0.40
1:E:318:SER:HA	1:E:335:ASN:OD1	2.22	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	108/111 (97%)	105 (97%)	2 (2%)	1 (1%)	14	14
1	C	108/111 (97%)	104 (96%)	3 (3%)	1 (1%)	14	14
1	E	108/111 (97%)	104 (96%)	3 (3%)	1 (1%)	14	14
1	G	108/111 (97%)	102 (94%)	5 (5%)	1 (1%)	14	14
2	B	24/30 (80%)	24 (100%)	0	0	100	100
2	D	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
2	F	25/30 (83%)	23 (92%)	2 (8%)	0	100	100
2	H	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
All	All	530/564 (94%)	509 (96%)	17 (3%)	4 (1%)	16	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	343	SER
1	G	342	LEU
1	E	342	LEU

### 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	93/96 (97%)	89 (96%)	4 (4%)	25	31
1	C	94/96 (98%)	90 (96%)	4 (4%)	25	31
1	E	94/96 (98%)	90 (96%)	4 (4%)	25	31
1	G	93/96 (97%)	88 (95%)	5 (5%)	18	22
2	B	18/24 (75%)	18 (100%)	0	100	100
2	D	20/24 (83%)	18 (90%)	2 (10%)	6	5
2	F	23/24 (96%)	21 (91%)	2 (9%)	8	7
2	H	23/24 (96%)	21 (91%)	2 (9%)	8	7
All	All	458/480 (95%)	435 (95%)	23 (5%)	20	25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	SER
1	A	418	THR
1	A	425	THR
1	A	426	ILE
1	C	351	ASN
1	C	418	THR
1	C	425	THR
1	C	426	ILE
2	D	143	ASN
2	D	150	THR
1	E	325	GLN
1	E	335	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	425	THR
1	E	426	ILE
2	F	143	ASN
2	F	150	THR
1	G	335	ASN
1	G	408	ASP
1	G	418	THR
1	G	425	THR
1	G	426	ILE
2	H	143	ASN
2	H	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	C	325	GLN
2	D	144	GLN
1	E	325	GLN
1	E	390	GLN
1	G	325	GLN
1	G	327	GLN
1	G	335	ASN
1	G	390	GLN
2	H	141	HIS
2	H	143	ASN

### 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

Of 13 ligands modelled in this entry, 9 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	A1CBG	E	501	-	36,43,43	0.67	0	51,64,64	1.12	3 (5%)
3	A1CBG	G	501	-	36,43,43	0.77	0	51,64,64	1.03	1 (1%)
3	A1CBG	A	501	-	36,43,43	0.71	1 (2%)	51,64,64	1.07	2 (3%)
3	A1CBG	C	501	-	36,43,43	0.73	0	51,64,64	0.99	2 (3%)

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	A1CBG	E	501	-	-	1/12/54/54	0/7/7/7
3	A1CBG	G	501	-	-	2/12/54/54	0/7/7/7
3	A1CBG	A	501	-	-	0/12/54/54	0/7/7/7
3	A1CBG	C	501	-	-	2/12/54/54	0/7/7/7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	A1CBG	C21-N4	-2.00	1.32	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	A1CBG	C19-N3-C16	4.31	109.13	104.04
3	E	501	A1CBG	C19-N3-C16	3.65	108.35	104.04
3	G	501	A1CBG	C19-N3-C16	3.28	107.92	104.04
3	E	501	A1CBG	C15-C14-C20	2.71	124.65	119.95
3	E	501	A1CBG	C23-N5-C24	2.56	127.90	125.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	A1CBG	C23-N5-C24	2.36	127.70	125.37
3	C	501	A1CBG	C14-C15-N3	-2.32	110.80	114.07
3	A	501	A1CBG	C13-C14-C20	-2.24	116.49	118.87

There are no chirality outliers.

All (5) torsion outliers are listed below:

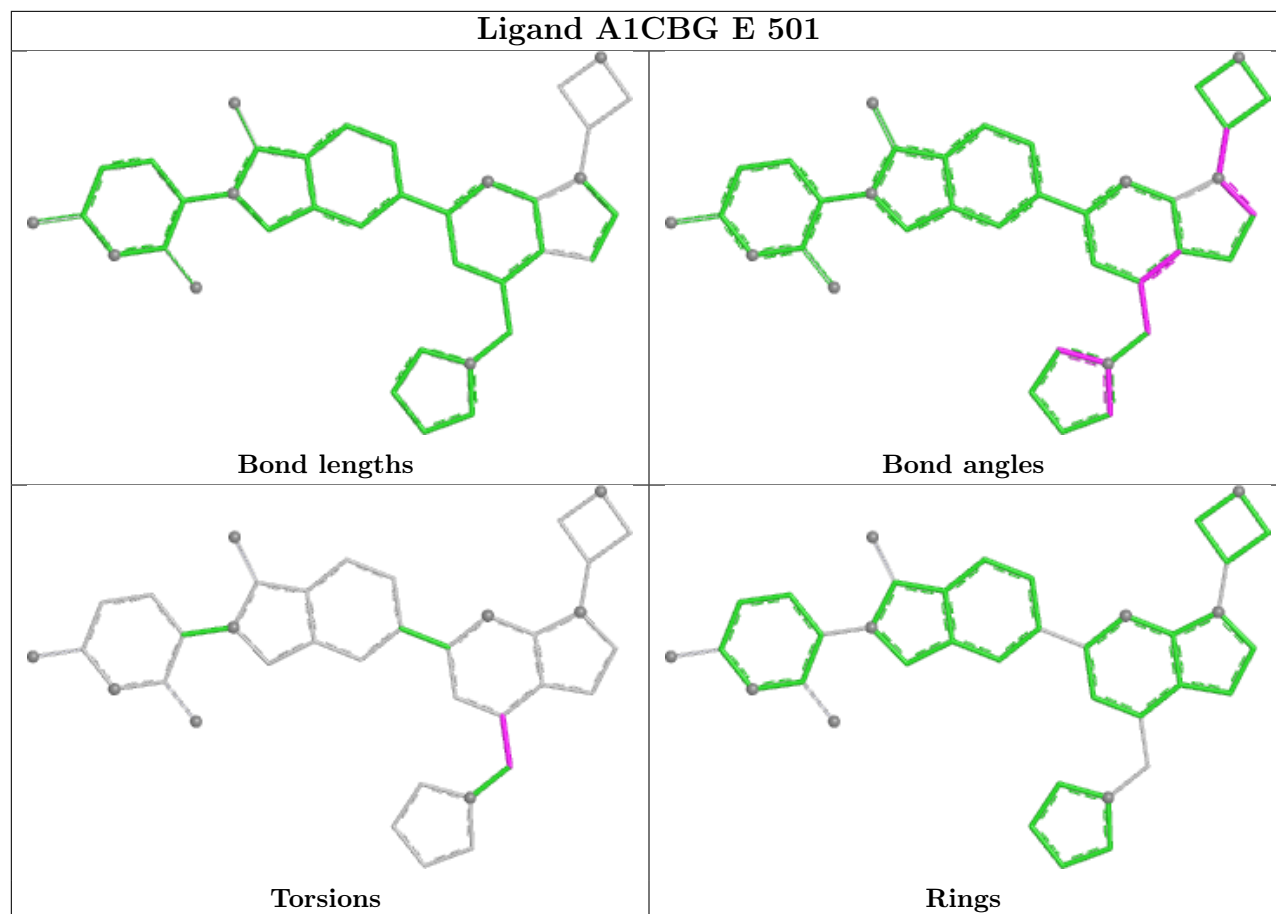
Mol	Chain	Res	Type	Atoms
3	C	501	A1CBG	C14-C15-N3-C16
3	E	501	A1CBG	C20-C14-C15-N3
3	G	501	A1CBG	C20-C14-C15-N3
3	C	501	A1CBG	C20-C14-C15-N3
3	G	501	A1CBG	C13-C14-C15-N3

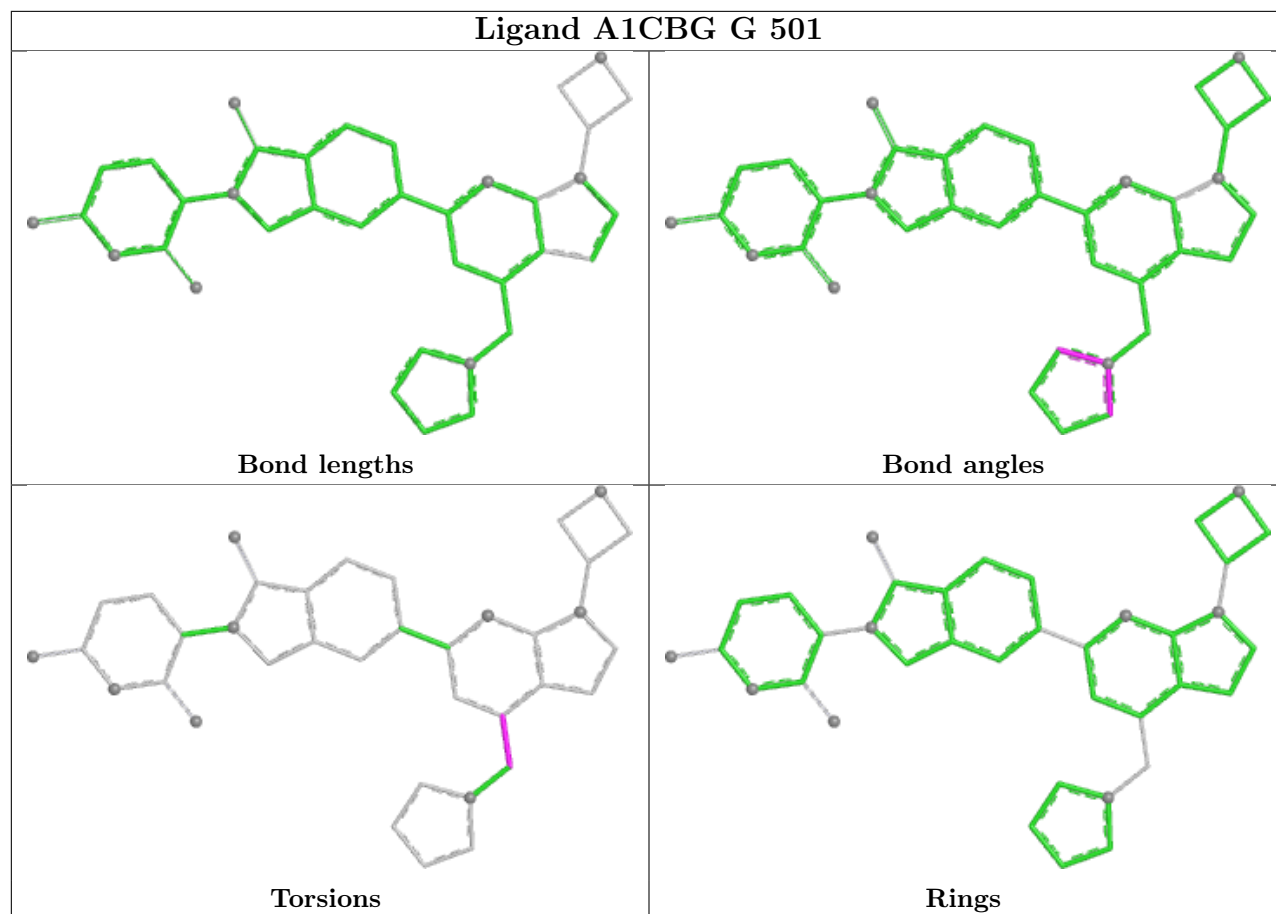
There are no ring outliers.

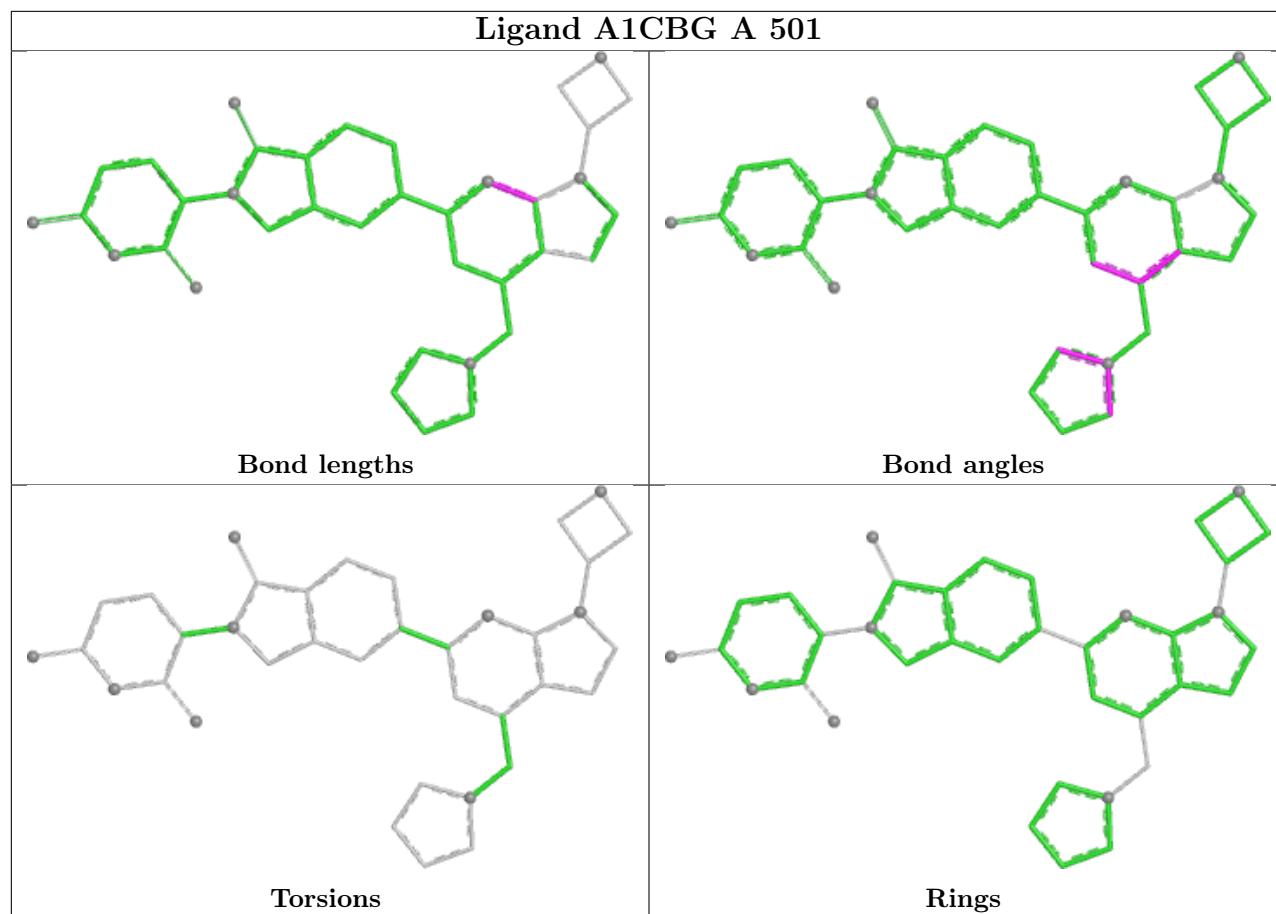
No monomer is involved in short contacts.

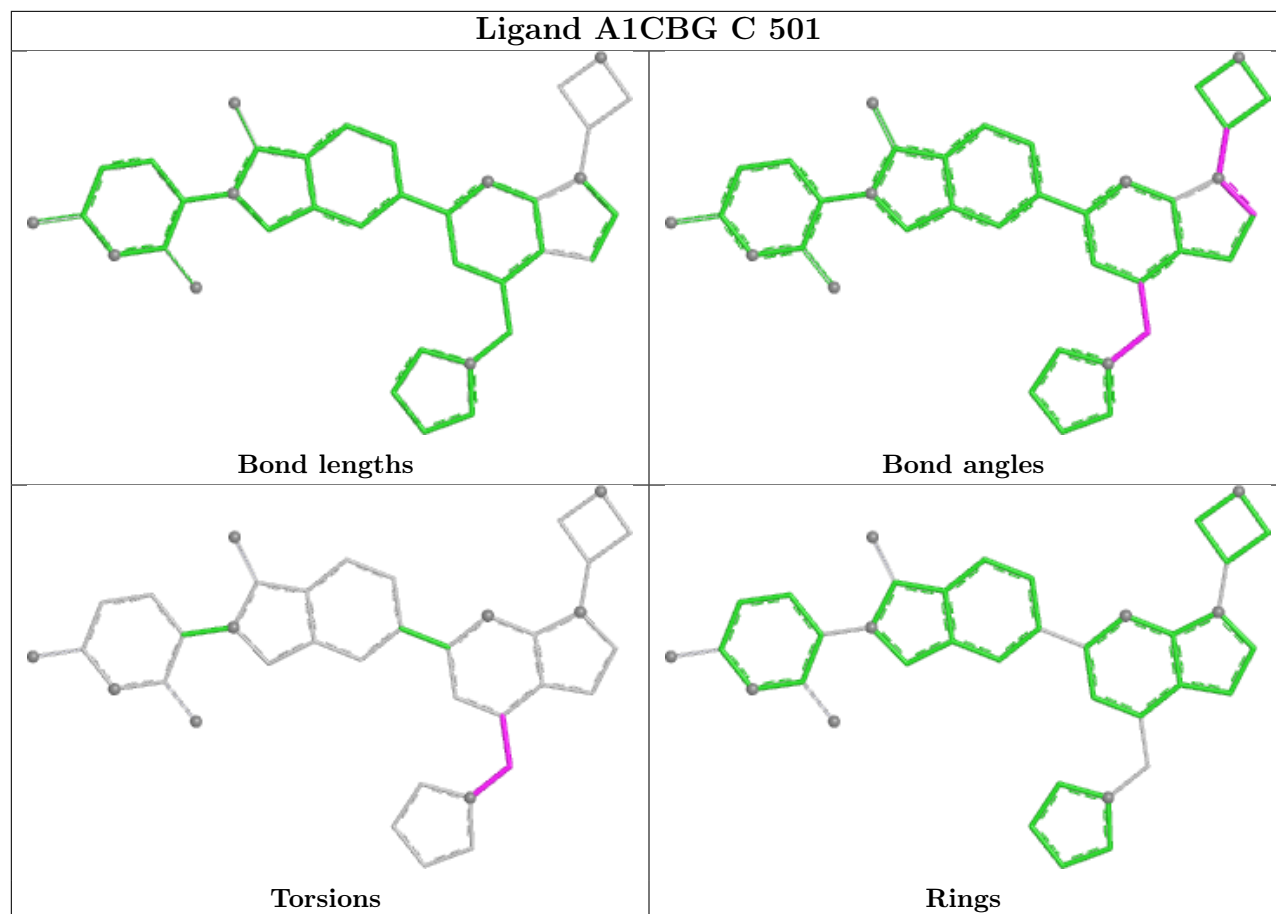
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand A1CBG E 501









## 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, 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	110/111 (99%)	0.51	6 (5%) 32 38	24, 34, 67, 80	0
1	C	110/111 (99%)	0.63	8 (7%) 22 28	23, 33, 65, 107	0
1	E	110/111 (99%)	0.58	11 (10%) 14 17	23, 32, 70, 120	0
1	G	110/111 (99%)	0.60	9 (8%) 19 24	23, 33, 71, 106	0
2	B	26/30 (86%)	0.92	4 (15%) 6 8	24, 38, 60, 65	0
2	D	26/30 (86%)	1.00	1 (3%) 44 52	31, 42, 54, 60	0
2	F	27/30 (90%)	0.99	2 (7%) 22 27	30, 42, 65, 72	0
2	H	27/30 (90%)	0.83	2 (7%) 22 27	26, 40, 58, 67	0
All	All	546/564 (96%)	0.65	43 (7%) 20 25	23, 34, 67, 120	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	342	LEU	6.2
1	C	317	PRO	6.1
1	E	317	PRO	4.7
1	G	317	PRO	4.3
1	A	340	LEU	4.2
1	C	342	LEU	4.2
1	G	426	ILE	4.0
1	G	340	LEU	3.8
1	C	426	ILE	3.7
2	B	150	THR	3.6
2	B	138	ARG	3.6
1	G	328	GLU	3.5
1	E	318	SER	3.5
1	C	318	SER	3.4
2	F	152	LYS	3.1
1	E	340	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	150	THR	2.9
1	G	425	THR	2.9
1	E	319	THR	2.8
1	G	318	SER	2.8
1	E	426	ILE	2.8
1	E	343	SER	2.8
2	B	163	SER	2.7
2	H	139	PRO	2.7
1	A	426	ILE	2.6
1	C	340	LEU	2.6
1	A	342	LEU	2.6
1	C	341	SER	2.6
1	E	371	ILE	2.5
1	G	329	THR	2.5
1	A	317	PRO	2.4
1	E	408	ASP	2.4
2	H	140	PHE	2.3
1	E	341	SER	2.3
1	A	344	GLY	2.3
1	G	424	PRO	2.2
1	G	343	SER	2.1
1	C	329	THR	2.1
1	A	343	SER	2.1
1	C	344	GLY	2.1
2	B	156	LEU	2.0
2	F	140	PHE	2.0
1	E	409	MET	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,



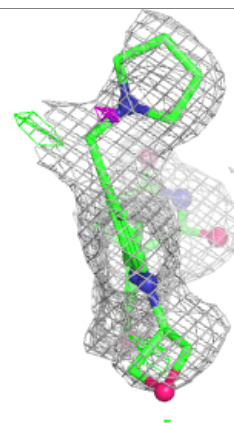
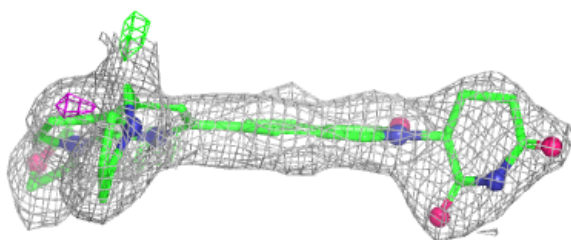
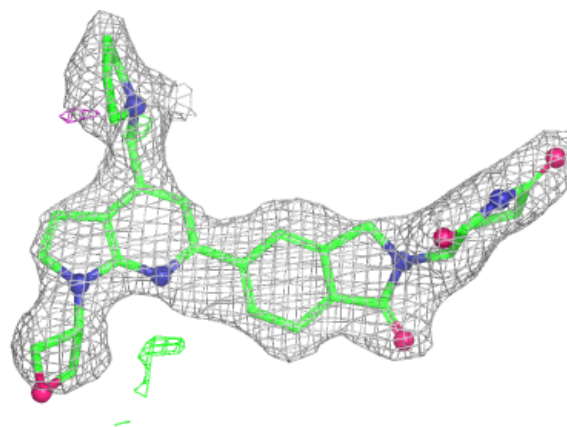
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	A1CBG	C	501	37/37	0.85	0.13	30,44,54,58	0
3	A1CBG	G	501	37/37	0.87	0.12	28,37,51,53	0
3	A1CBG	E	501	37/37	0.90	0.11	22,39,58,61	0
3	A1CBG	A	501	37/37	0.90	0.10	30,41,48,51	0
4	ZN	G	502	1/1	0.98	0.03	49,49,49,49	0
4	ZN	C	502	1/1	0.99	0.03	32,32,32,32	0
4	ZN	E	502	1/1	0.99	0.02	28,28,28,28	0
4	ZN	A	502	1/1	0.99	0.02	33,33,33,33	0
4	ZN	G	503	1/1	0.99	0.02	30,30,30,30	0
4	ZN	F	201	1/1	1.00	0.01	32,32,32,32	0
4	ZN	D	201	1/1	1.00	0.01	29,29,29,29	0
4	ZN	B	201	1/1	1.00	0.01	28,28,28,28	0
4	ZN	H	201	1/1	1.00	0.01	27,27,27,27	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.

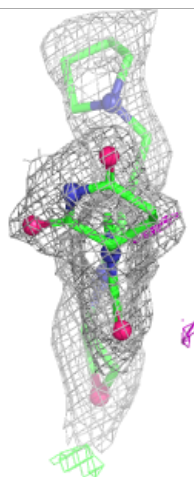
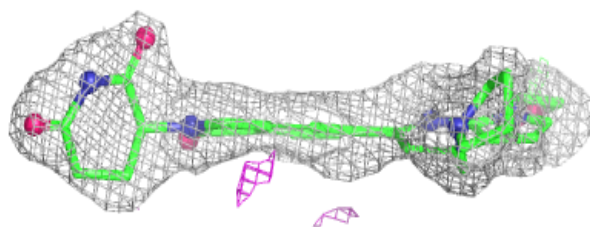
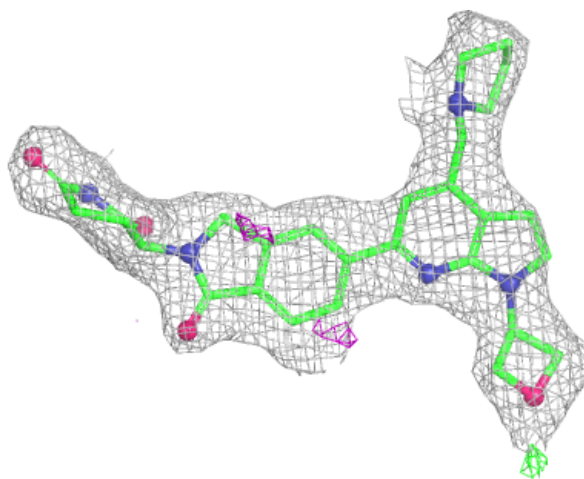
#### Electron density around A1CBG C 501:

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)



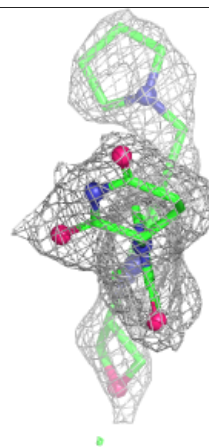
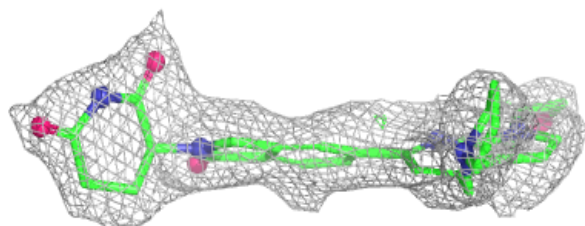
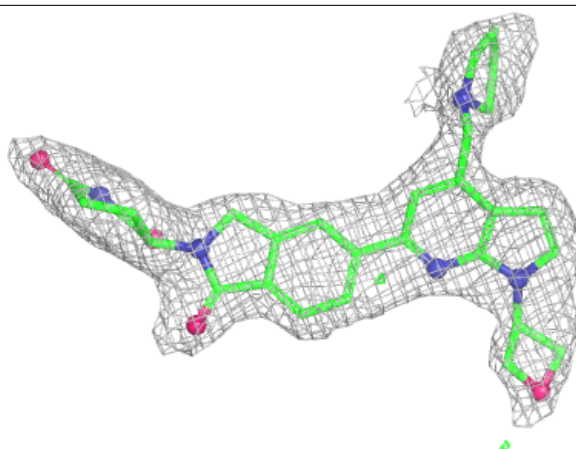
**Electron density around A1CBG G 501:**

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



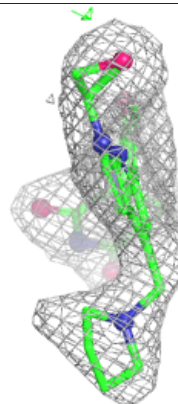
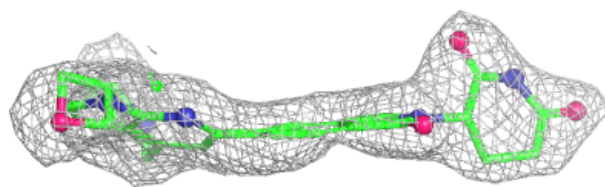
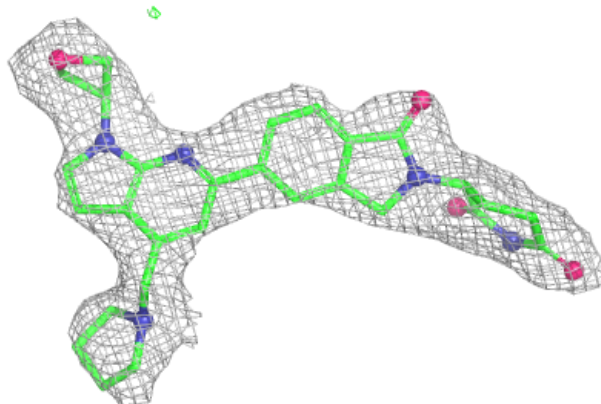
**Electron density around A1CBG E 501:**

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



**Electron density around A1CBG 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 [i](#)

There are no such residues in this entry.