



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:32 PM UTC

PDB ID : 9CUO / pdb\_00009cuo  
Title : Crystal structure of CRBN with compound 3  
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Deposited on : 2024-07-26  
Resolution : 1.60 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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

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



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Mol	Chain	Length	Quality of chain
1	F	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	504	-	-	X	-
4	SO4	F	503	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5207 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
			Total	C	N	O	S			
1	A	96	790	507	134	141	8	0	4	0
1	B	92	755	484	128	135	8	0	3	0
1	C	96	784	502	132	142	8	0	3	0
1	D	93	776	495	132	141	8	0	5	0
1	E	95	780	499	132	142	7	0	4	0
1	F	96	784	502	133	142	7	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	SER	-	expression tag	UNP Q96SW2
A	316	GLY	-	expression tag	UNP Q96SW2
A	317	SER	-	expression tag	UNP Q96SW2
A	318	PRO	-	expression tag	UNP Q96SW2
B	315	SER	-	expression tag	UNP Q96SW2
B	316	GLY	-	expression tag	UNP Q96SW2
B	317	SER	-	expression tag	UNP Q96SW2
B	318	PRO	-	expression tag	UNP Q96SW2
C	315	SER	-	expression tag	UNP Q96SW2
C	316	GLY	-	expression tag	UNP Q96SW2
C	317	SER	-	expression tag	UNP Q96SW2
C	318	PRO	-	expression tag	UNP Q96SW2
D	315	SER	-	expression tag	UNP Q96SW2
D	316	GLY	-	expression tag	UNP Q96SW2
D	317	SER	-	expression tag	UNP Q96SW2
D	318	PRO	-	expression tag	UNP Q96SW2
E	315	SER	-	expression tag	UNP Q96SW2

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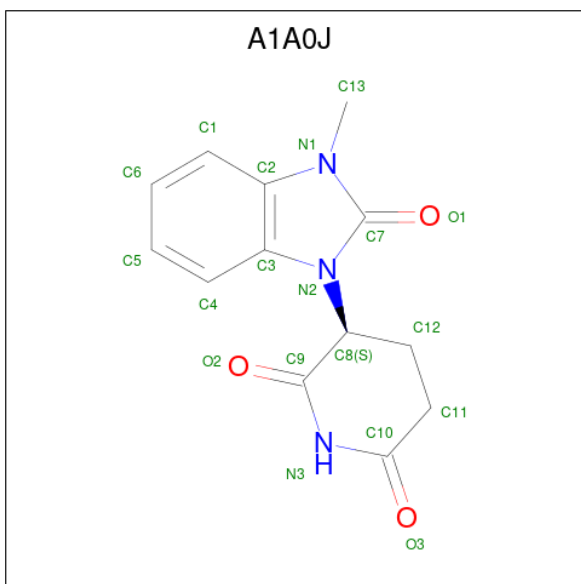
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Chain	Residue	Modelled	Actual	Comment	Reference
E	316	GLY	-	expression tag	UNP Q96SW2
E	317	SER	-	expression tag	UNP Q96SW2
E	318	PRO	-	expression tag	UNP Q96SW2
F	315	SER	-	expression tag	UNP Q96SW2
F	316	GLY	-	expression tag	UNP Q96SW2
F	317	SER	-	expression tag	UNP Q96SW2
F	318	PRO	-	expression tag	UNP Q96SW2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

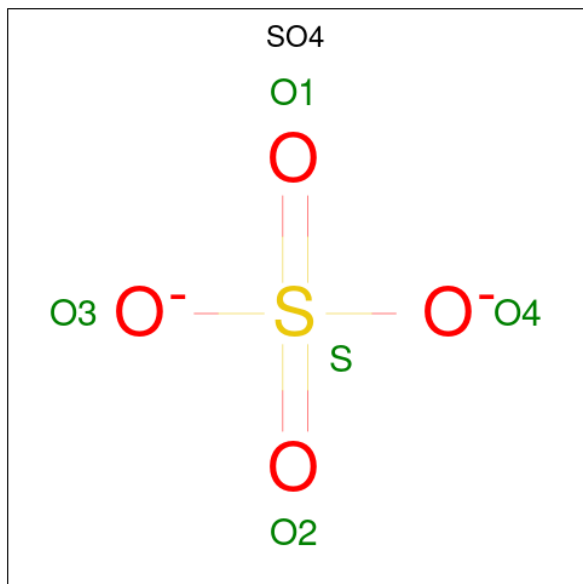
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is (3S)-3-(3-methyl-2-oxo-2,3-dihydro-1H-1,3-benzimidazol-1-yl)piperidin e-2,6-dione (CCD ID: A1A0J) (formula: C<sub>13</sub>H<sub>13</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	13	3	3		
3	B	1	Total	C	N	O	0	0
			19	13	3	3		
3	C	1	Total	C	N	O	0	0
			19	13	3	3		
3	D	1	Total	C	N	O	0	0
			19	13	3	3		
3	E	1	Total	C	N	O	0	0
			19	13	3	3		
3	F	1	Total	C	N	O	0	0
			19	13	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



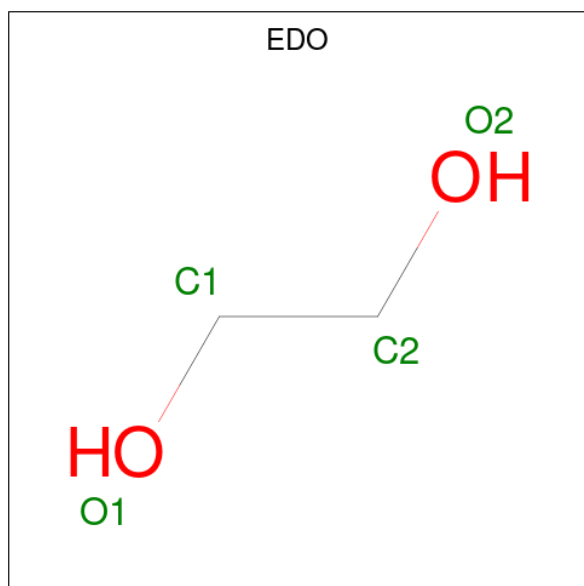
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

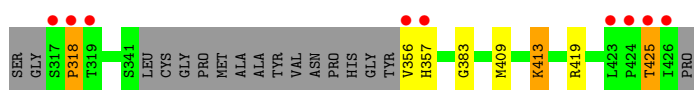
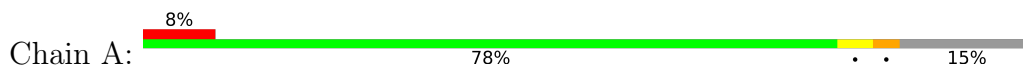
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	49	Total O 49 49	0	0
6	B	48	Total O 48 48	0	0
6	C	58	Total O 58 58	0	0
6	D	55	Total O 55 55	0	0
6	E	43	Total O 43 43	0	0
6	F	52	Total O 52 52	0	0

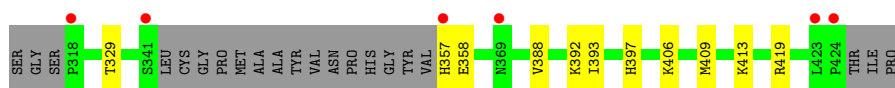
### 3 Residue-property plots [i](#)

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.

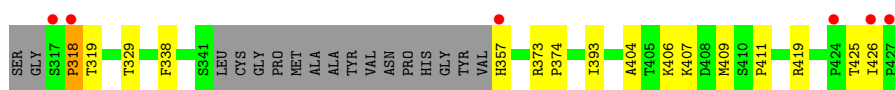
- Molecule 1: Protein cereblon



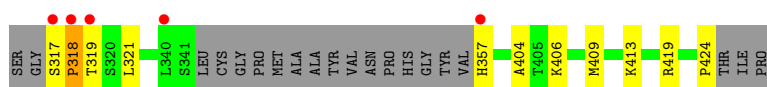
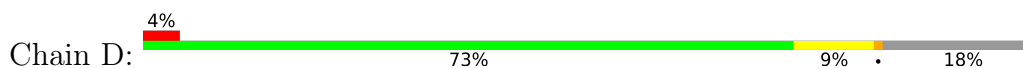
- Molecule 1: Protein cereblon



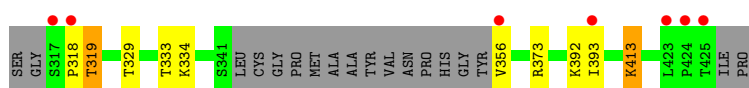
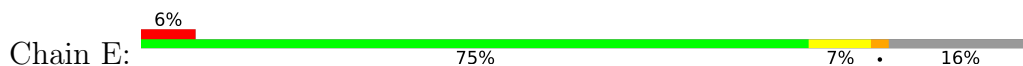
- Molecule 1: Protein cereblon




- Molecule 1: Protein cereblon

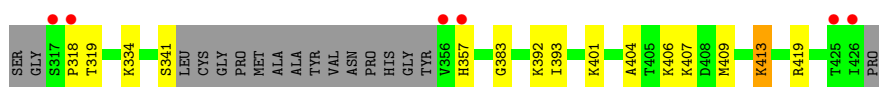


- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon

Chain F: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.47Å 141.50Å 141.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.72 – 1.60 42.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.72-1.60) 100.0 (42.72-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.155 , 0.205 0.162 , 0.208	Depositor DCC
$R_{free}$ test set	4660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.007 for -h,l,k 0.014 for l,-k,h 0.013 for -k,-h,-l 0.128 for -k,-l,h 0.128 for l,-h,-k	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.86 % 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 9.0568e-06. 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: EDO, SO4, ZN, A1A0J

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	0.98	0/814	1.11	2/1102 (0.2%)
1	B	0.92	0/775	1.09	1/1047 (0.1%)
1	C	0.97	0/805	1.13	4/1089 (0.4%)
1	D	0.94	0/796	1.07	2/1076 (0.2%)
1	E	0.95	0/807	1.06	2/1094 (0.2%)
1	F	0.95	0/804	1.11	0/1089
All	All	0.95	0/4801	1.09	11/6497 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	425	THR	CA-C-N	6.56	125.58	120.33
1	C	425	THR	C-N-CA	6.56	125.58	120.33
1	D	318	PRO	CA-C-N	6.10	128.96	120.29
1	D	318	PRO	C-N-CA	6.10	128.96	120.29
1	A	318	PRO	CA-C-N	5.69	128.36	120.29
1	A	318	PRO	C-N-CA	5.69	128.36	120.29
1	C	318	PRO	CA-C-N	5.46	128.04	120.29
1	C	318	PRO	C-N-CA	5.46	128.04	120.29
1	E	356	VAL	CA-C-N	5.07	127.08	120.28
1	E	356	VAL	C-N-CA	5.07	127.08	120.28
1	B	358	GLU	CB-CG-CD	5.02	121.13	112.60

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	790	0	788	6	0
1	B	755	0	750	12	0
1	C	784	0	779	11	0
1	D	776	0	765	12	0
1	E	780	0	770	11	0
1	F	784	0	780	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
3	F	19	0	0	0	0
4	A	10	0	0	1	0
4	B	15	0	0	2	0
4	C	15	0	0	0	0
4	D	10	0	0	3	0
4	E	5	0	0	0	0
4	F	10	0	0	2	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	D	12	0	18	0	0
5	E	24	0	36	4	0
5	F	4	0	6	0	0
6	A	49	0	0	1	0
6	B	48	0	0	3	0
6	C	58	0	0	2	0
6	D	55	0	0	5	0
6	E	43	0	0	2	0
6	F	52	0	0	5	0
All	All	5207	0	4704	72	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 7.

All (72) 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)
6:C:636:HOH:O	5:E:507:EDO:H21	1.69	0.92
1:F:404:ALA:HB1	1:F:409:MET:HE3	1.59	0.82
1:F:392:LYS:HG3	1:F:393:ILE:HD12	1.64	0.79
4:F:503:SO4:O2	6:F:601:HOH:O	2.09	0.70
1:B:329:THR:HG21	1:B:393:ILE:HD13	1.75	0.69
1:E:392:LYS:HG3	1:E:393:ILE:HD12	1.77	0.67
1:C:404:ALA:HB1	1:C:409[B]:MET:HE3	1.77	0.65
1:D:404:ALA:HB1	1:D:409[B]:MET:HE3	1.79	0.64
1:D:413:LYS:HG3	6:D:630:HOH:O	1.97	0.64
1:C:373:ARG:HG2	1:C:374:PRO:HD2	1.81	0.63
4:D:504:SO4:O1	1:F:413:LYS:CE	2.47	0.63
1:D:413:LYS:CG	6:D:630:HOH:O	2.47	0.62
1:E:392:LYS:CG	1:E:393:ILE:HD12	2.30	0.61
4:D:504:SO4:O1	1:F:413:LYS:HE3	1.99	0.61
1:B:392:LYS:HG3	1:B:393:ILE:HD12	1.81	0.60
1:C:318:PRO:HA	1:C:426:ILE:HA	1.84	0.59
1:F:318:PRO:O	1:F:334:LYS:HE3	2.03	0.58
1:B:392:LYS:CG	1:B:393:ILE:HD12	2.34	0.57
1:C:329:THR:HG21	1:C:393:ILE:HD13	1.88	0.56
1:B:413:LYS:HE3	6:C:625:HOH:O	2.05	0.56
1:E:329:THR:HG21	1:E:393:ILE:HD13	1.86	0.56
1:C:406:LYS:HB2	1:C:409[B]:MET:HE2	1.89	0.55
1:A:357:HIS:O	1:A:419:ARG:NE	2.41	0.54
1:F:404:ALA:HB1	1:F:409:MET:CE	2.33	0.54
5:E:505:EDO:O1	6:E:601:HOH:O	2.05	0.54
1:E:413:LYS:HD2	1:E:413:LYS:C	2.34	0.53
1:B:393:ILE:HD12	1:B:393:ILE:N	2.25	0.52
1:F:406:LYS:H	1:F:409:MET:HE2	1.73	0.52
1:C:357:HIS:O	1:C:419:ARG:NE	2.38	0.52
1:B:357:HIS:O	1:B:419:ARG:NE	2.43	0.52
1:D:413:LYS:CE	6:D:639:HOH:O	2.58	0.51
1:A:356:VAL:N	4:A:504:SO4:O4	2.44	0.51
1:F:357:HIS:O	1:F:419:ARG:NE	2.35	0.50
1:D:357:HIS:O	1:D:419:ARG:NE	2.45	0.49
1:F:401:LYS:CE	6:F:638:HOH:O	2.61	0.49
1:F:413:LYS:HG2	6:F:620:HOH:O	2.12	0.49
1:B:406:LYS:HB2	1:B:409[B]:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:HG13	1:B:397:HIS:CD2	2.48	0.48
4:B:503:SO4:O2	1:C:411:PRO:HA	2.12	0.48
1:C:393:ILE:HD12	1:C:393:ILE:N	2.28	0.48
1:B:413:LYS:CE	6:B:604:HOH:O	2.61	0.48
1:A:383:GLY:O	1:A:409[B]:MET:HE1	2.13	0.47
1:D:413:LYS:HE3	6:D:639:HOH:O	2.14	0.47
1:E:318:PRO:O	1:E:334:LYS:HE3	2.15	0.47
1:B:329:THR:CG2	1:B:393:ILE:HD13	2.43	0.46
1:F:406:LYS:HB2	1:F:409:MET:HE2	1.98	0.46
1:B:413:LYS:NZ	6:B:604:HOH:O	2.49	0.46
1:E:393:ILE:HD12	1:E:393:ILE:N	2.31	0.46
1:F:401:LYS:HE3	6:F:638:HOH:O	2.14	0.45
4:B:505:SO4:O1	1:C:338:PHE:HA	2.17	0.45
1:C:373:ARG:HG2	1:C:374:PRO:CD	2.46	0.45
1:F:319:THR:CG2	6:F:625:HOH:O	2.64	0.45
1:F:404:ALA:CB	1:F:409:MET:HE3	2.40	0.44
1:D:317:SER:N	1:D:318:PRO:HD3	2.33	0.43
1:B:413:LYS:HE2	6:B:604:HOH:O	2.18	0.43
1:E:333:THR:CG2	6:E:602:HOH:O	2.66	0.43
1:F:383:GLY:O	1:F:409:MET:HE1	2.19	0.42
1:D:317:SER:N	1:D:318:PRO:CD	2.82	0.42
1:D:318:PRO:HB2	1:D:424:PRO:HG3	2.01	0.42
1:D:321:LEU:HD23	1:D:424:PRO:HD2	2.02	0.42
4:D:504:SO4:S	1:F:413:LYS:HE2	2.60	0.42
1:D:413:LYS:HE2	6:D:639:HOH:O	2.18	0.42
1:A:357:HIS:HA	6:A:641:HOH:O	2.20	0.42
1:E:413:LYS:HE3	4:F:503:SO4:O3	2.20	0.41
1:C:329:THR:CG2	1:C:393:ILE:HD13	2.50	0.41
1:A:318:PRO:HA	1:A:425:THR:O	2.20	0.41
1:F:406:LYS:N	1:F:409:MET:HE2	2.36	0.41
1:E:319:THR:HG22	5:E:508:EDO:H11	2.02	0.41
1:E:392:LYS:HG2	1:E:393:ILE:HD12	2.02	0.40
1:E:319:THR:CG2	5:E:508:EDO:H11	2.50	0.40
1:D:406:LYS:HB2	1:D:409[B]:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/113 (85%)	95 (99%)	1 (1%)	0	100	100
1	B	91/113 (80%)	90 (99%)	1 (1%)	0	100	100
1	C	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
1	D	94/113 (83%)	92 (98%)	2 (2%)	0	100	100
1	E	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
1	F	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
All	All	566/678 (84%)	555 (98%)	11 (2%)	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	90/98 (92%)	87 (97%)	3 (3%)	33	12
1	B	85/98 (87%)	85 (100%)	0	100	100
1	C	89/98 (91%)	87 (98%)	2 (2%)	45	22
1	D	88/98 (90%)	87 (99%)	1 (1%)	65	46
1	E	89/98 (91%)	86 (97%)	3 (3%)	32	11
1	F	89/98 (91%)	86 (97%)	3 (3%)	32	11
All	All	530/588 (90%)	518 (98%)	12 (2%)	45	20

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413[A]	LYS
1	A	413[B]	LYS
1	A	425	THR
1	C	319	THR
1	C	407	LYS
1	D	319	THR
1	E	319	THR
1	E	373	ARG
1	E	413	LYS
1	F	341	SER
1	F	407	LYS
1	F	413	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	A	378	HIS
1	A	390	GLN
1	B	335	ASN
1	B	390	GLN
1	B	412	GLN
1	C	327	GLN
1	C	335	ASN
1	D	327	GLN
1	D	335	ASN
1	E	335	ASN
1	F	327	GLN
1	F	335	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 [i](#)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	A1A0J	E	502	-	21,21,21	0.60	0	28,31,31	0.73	1 (3%)
5	EDO	D	507	-	3,3,3	0.14	0	2,2,2	0.27	0
4	SO4	E	503	-	4,4,4	0.41	0	6,6,6	0.17	0
5	EDO	D	505	-	3,3,3	0.37	0	2,2,2	0.34	0
4	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.58	0
5	EDO	E	505	-	3,3,3	0.17	0	2,2,2	0.10	0
3	A1A0J	D	502	-	21,21,21	0.47	0	28,31,31	0.69	0
4	SO4	F	504	-	4,4,4	0.32	0	6,6,6	0.17	0
5	EDO	F	505	-	3,3,3	0.32	0	2,2,2	0.28	0
5	EDO	E	507	-	3,3,3	0.37	0	2,2,2	0.75	0
4	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	503	-	4,4,4	0.37	0	6,6,6	0.22	0
4	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.16	0
5	EDO	E	504	-	3,3,3	0.18	0	2,2,2	0.04	0
4	SO4	F	503	-	4,4,4	0.44	0	6,6,6	0.68	0
4	SO4	B	504	-	4,4,4	0.29	0	6,6,6	0.11	0
3	A1A0J	C	502	-	21,21,21	0.45	0	28,31,31	0.64	0
5	EDO	D	506	-	3,3,3	0.27	0	2,2,2	0.19	0
3	A1A0J	B	502	-	21,21,21	0.45	0	28,31,31	0.69	1 (3%)
4	SO4	C	503	-	4,4,4	0.34	0	6,6,6	0.12	0
5	EDO	E	508	-	3,3,3	0.12	0	2,2,2	0.16	0
4	SO4	B	503	-	4,4,4	0.43	0	6,6,6	0.35	0
5	EDO	E	506	-	3,3,3	1.54	0	2,2,2	1.18	0
4	SO4	B	505	-	4,4,4	0.31	0	6,6,6	0.10	0
3	A1A0J	A	502	-	21,21,21	0.54	0	28,31,31	0.68	0
4	SO4	D	504	-	4,4,4	0.34	0	6,6,6	0.52	0
4	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	505	-	3,3,3	0.19	0	2,2,2	0.25	0
3	A1A0J	F	502	-	21,21,21	0.51	0	28,31,31	0.77	1 (3%)
5	EDO	B	506	-	3,3,3	0.08	0	2,2,2	0.38	0
5	EDO	E	509	-	3,3,3	0.23	0	2,2,2	0.25	0

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	A1A0J	E	502	-	-	0/4/17/17	0/3/3/3
5	EDO	D	507	-	-	1/1/1/1	-
3	A1A0J	C	502	-	-	0/4/17/17	0/3/3/3
5	EDO	D	506	-	-	0/1/1/1	-
5	EDO	D	505	-	-	0/1/1/1	-
5	EDO	E	506	-	-	0/1/1/1	-
5	EDO	E	507	-	-	0/1/1/1	-
3	A1A0J	B	502	-	-	0/4/17/17	0/3/3/3
5	EDO	A	505	-	-	0/1/1/1	-
3	A1A0J	F	502	-	-	0/4/17/17	0/3/3/3
5	EDO	E	509	-	-	1/1/1/1	-
5	EDO	E	505	-	-	1/1/1/1	-
5	EDO	B	506	-	-	1/1/1/1	-
5	EDO	E	508	-	-	1/1/1/1	-
5	EDO	E	504	-	-	1/1/1/1	-
3	A1A0J	D	502	-	-	0/4/17/17	0/3/3/3
3	A1A0J	A	502	-	-	0/4/17/17	0/3/3/3
5	EDO	F	505	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	F	502	A1A0J	C9-C8-N2	-2.39	106.94	109.08
3	E	502	A1A0J	C13-N1-C7	2.25	125.56	123.59
3	B	502	A1A0J	C13-N1-C7	2.25	125.56	123.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

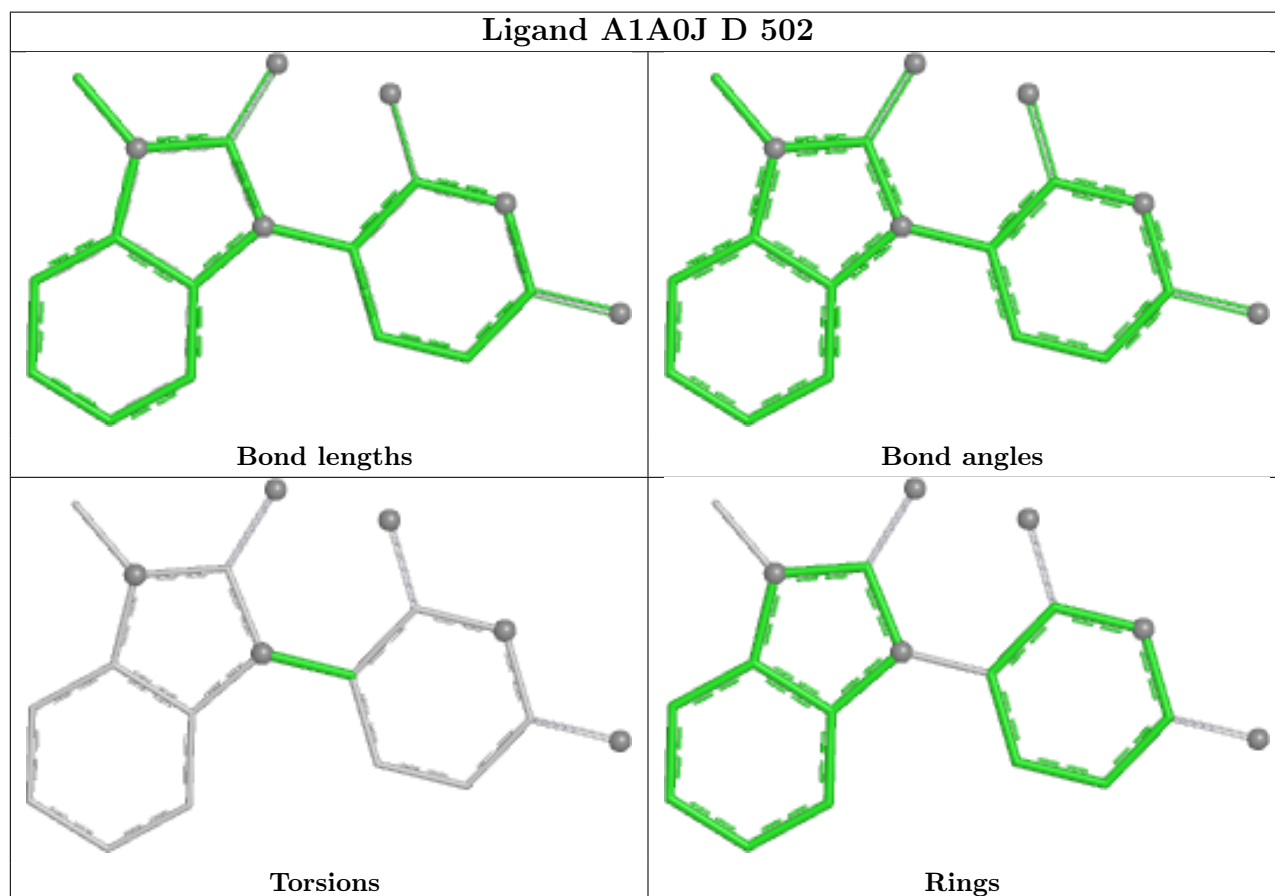
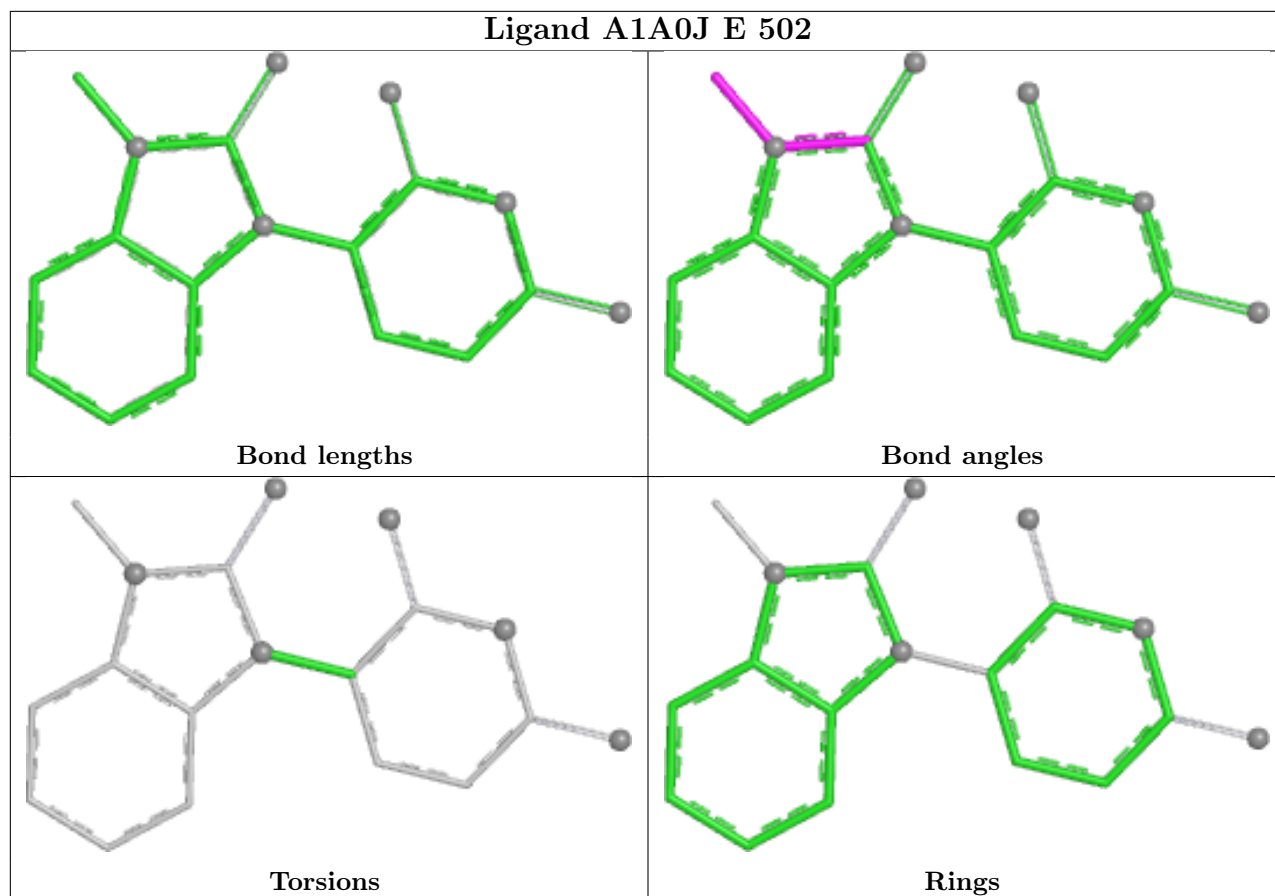
Mol	Chain	Res	Type	Atoms
5	B	506	EDO	O1-C1-C2-O2
5	E	509	EDO	O1-C1-C2-O2
5	E	504	EDO	O1-C1-C2-O2
5	E	505	EDO	O1-C1-C2-O2
5	E	508	EDO	O1-C1-C2-O2
5	D	507	EDO	O1-C1-C2-O2

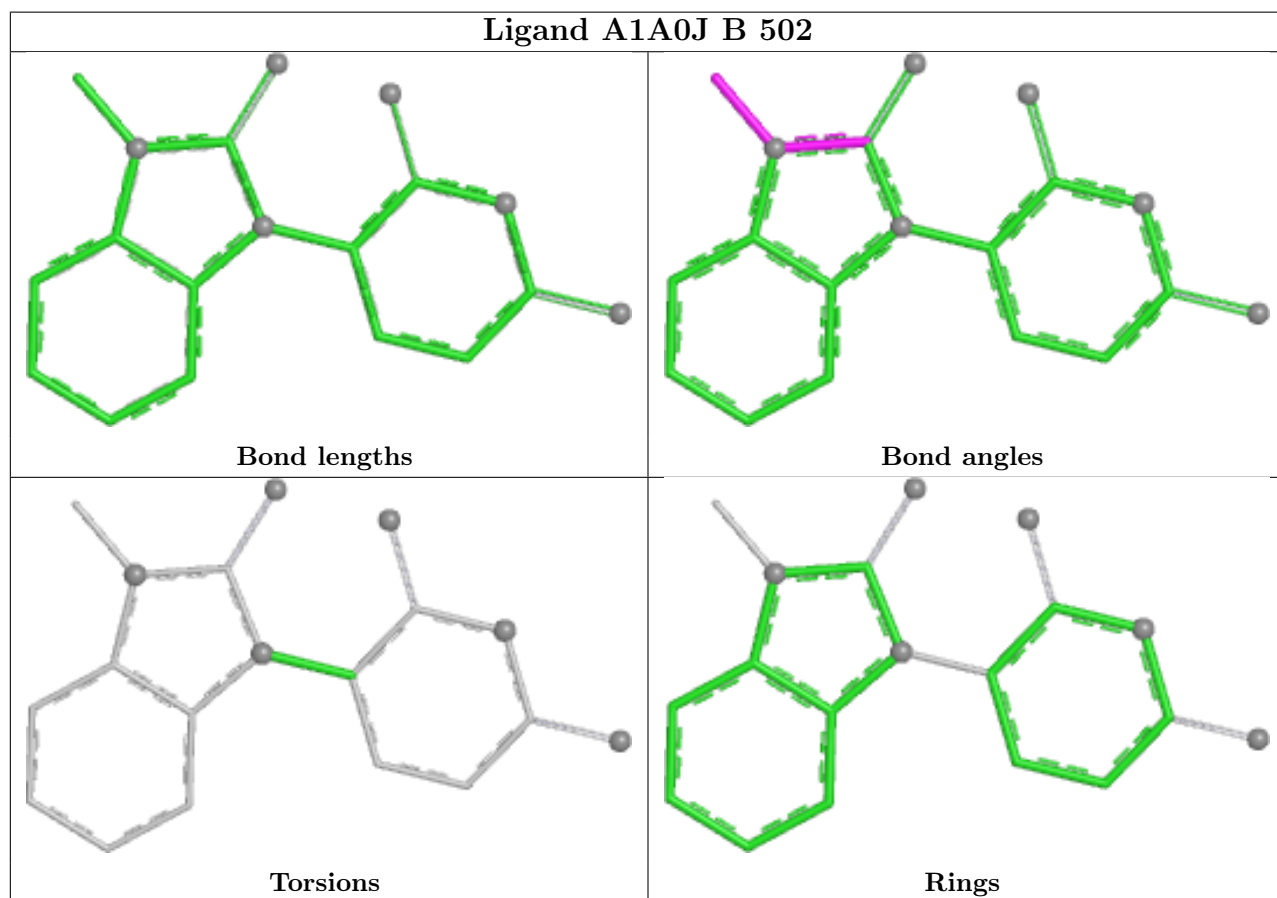
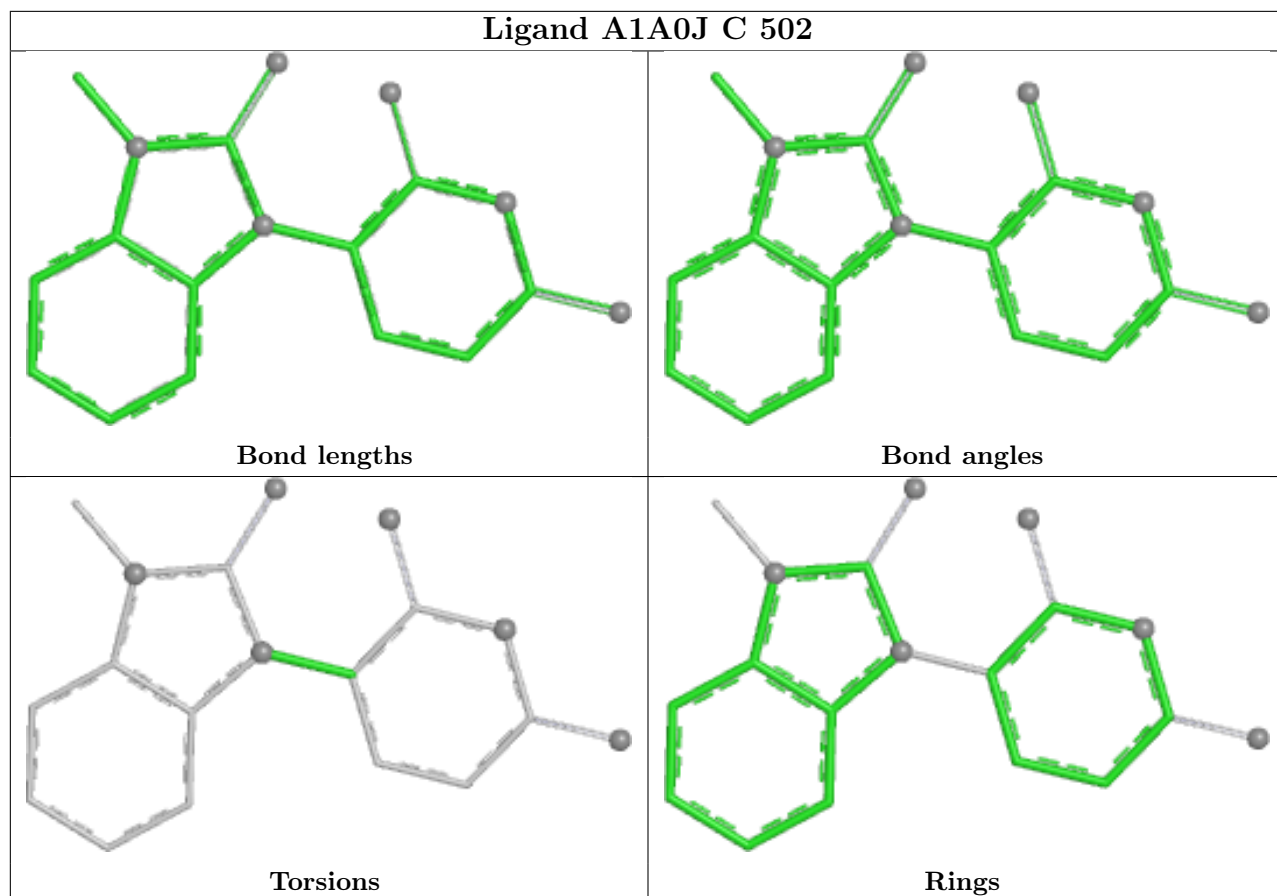
There are no ring outliers.

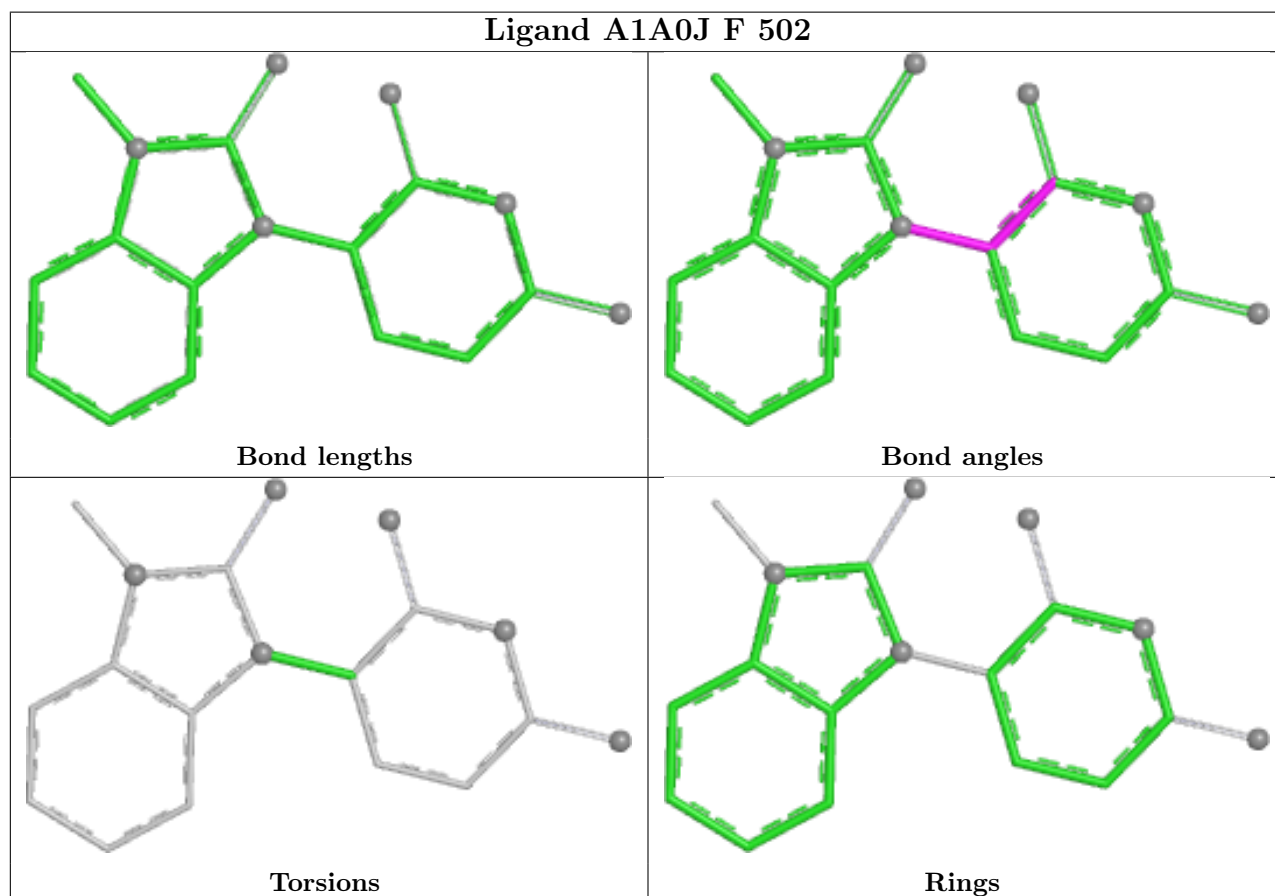
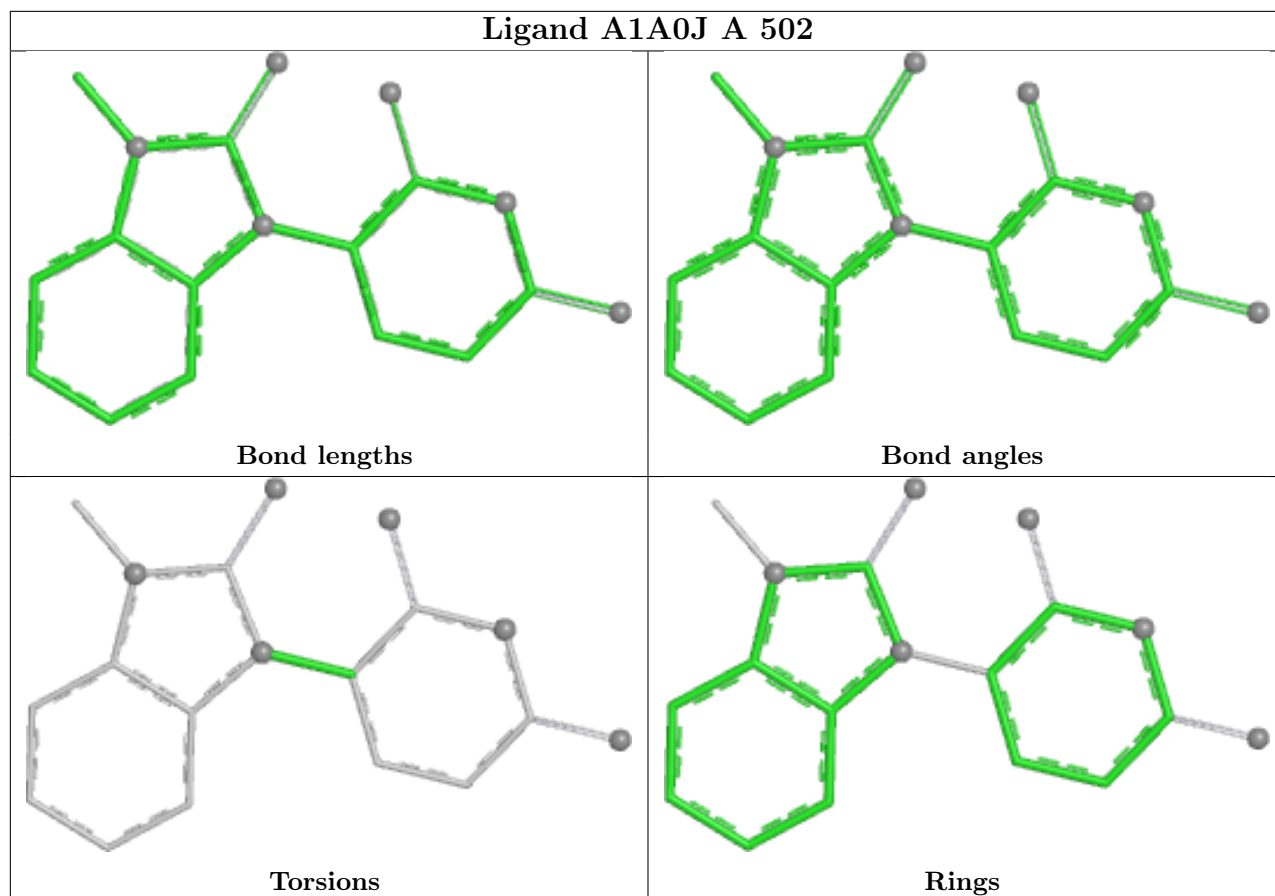
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	505	EDO	1	0
5	E	507	EDO	1	0
4	A	504	SO4	1	0
4	F	503	SO4	2	0
5	E	508	EDO	2	0
4	B	503	SO4	1	0
4	B	505	SO4	1	0
4	D	504	SO4	3	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	96/113 (84%)	0.58	9 (9%) 14 14	10, 28, 57, 80	4 (4%)
1	B	92/113 (81%)	0.49	6 (6%) 25 25	11, 28, 49, 77	3 (3%)
1	C	96/113 (84%)	0.34	6 (6%) 26 26	9, 26, 56, 75	3 (3%)
1	D	93/113 (82%)	0.47	5 (5%) 31 32	9, 25, 48, 78	5 (5%)
1	E	95/113 (84%)	0.52	7 (7%) 20 21	10, 27, 54, 85	4 (4%)
1	F	96/113 (84%)	0.43	6 (6%) 26 26	10, 27, 51, 79	3 (3%)
All	All	568/678 (83%)	0.47	39 (6%) 23 23	9, 27, 55, 85	22 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	ILE	7.0
1	E	318	PRO	6.8
1	F	356	VAL	5.8
1	A	356	VAL	4.7
1	F	317	SER	4.5
1	E	424	PRO	4.4
1	F	426	ILE	4.3
1	C	426	ILE	4.2
1	E	317	SER	4.1
1	F	318	PRO	4.1
1	E	356	VAL	3.9
1	E	425	THR	3.9
1	B	357	HIS	3.5
1	B	341	SER	3.5
1	D	318	PRO	3.5
1	B	318	PRO	3.4
1	C	317	SER	3.3
1	D	317	SER	3.3
1	A	424	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	425	THR	3.1
1	C	318	PRO	3.1
1	A	319	THR	3.0
1	A	357	HIS	2.8
1	D	357	HIS	2.7
1	D	319	THR	2.7
1	F	357	HIS	2.7
1	C	357	HIS	2.6
1	A	423	LEU	2.5
1	C	424	PRO	2.5
1	A	425	THR	2.5
1	C	427	PRO	2.4
1	B	423	LEU	2.4
1	D	340	LEU	2.3
1	E	423	LEU	2.3
1	A	318	PRO	2.3
1	B	424	PRO	2.2
1	A	317	SER	2.2
1	B	369	ASN	2.1
1	E	393	ILE	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
5	EDO	E	508	4/4	0.77	0.18	34,44,50,50	0
5	EDO	E	507	4/4	0.79	0.17	41,44,44,52	0
5	EDO	E	505	4/4	0.79	0.16	41,46,46,55	0

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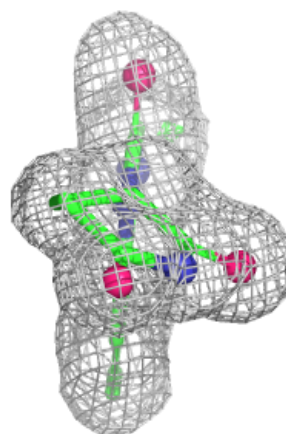
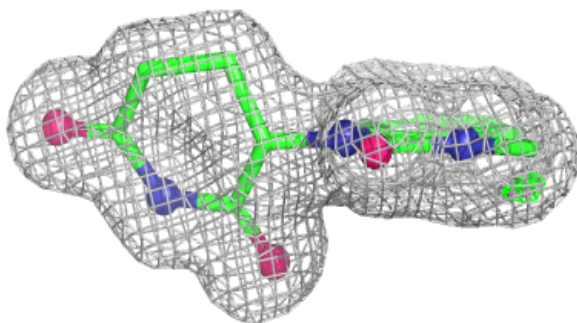
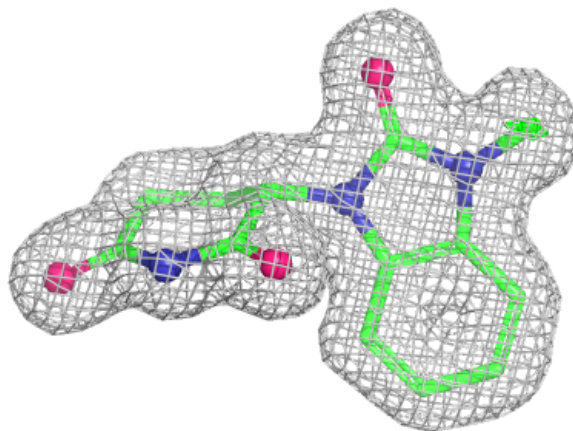
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	505	5/5	0.81	0.13	68,70,73,82	0
5	EDO	B	506	4/4	0.84	0.13	33,34,34,41	0
5	EDO	F	505	4/4	0.84	0.15	34,36,37,41	0
5	EDO	E	506	4/4	0.86	0.14	35,36,42,44	0
5	EDO	D	506	4/4	0.86	0.13	31,40,46,51	0
5	EDO	E	509	4/4	0.87	0.15	27,42,48,52	0
5	EDO	E	504	4/4	0.87	0.12	34,35,36,36	0
5	EDO	D	507	4/4	0.88	0.13	36,42,46,47	0
4	SO4	A	504	5/5	0.91	0.10	50,54,61,68	0
5	EDO	A	505	4/4	0.92	0.10	32,35,37,38	0
4	SO4	C	505	5/5	0.92	0.09	45,50,55,59	0
5	EDO	D	505	4/4	0.92	0.10	28,32,35,38	0
4	SO4	F	503	5/5	0.93	0.09	31,31,36,37	0
4	SO4	F	504	5/5	0.93	0.07	46,48,59,60	0
4	SO4	D	504	5/5	0.94	0.09	30,30,32,42	0
4	SO4	A	503	5/5	0.94	0.09	30,31,33,41	0
4	SO4	B	504	5/5	0.94	0.08	44,45,49,53	0
3	A1A0J	E	502	19/19	0.95	0.07	23,27,33,34	0
3	A1A0J	F	502	19/19	0.96	0.07	21,24,29,29	0
3	A1A0J	D	502	19/19	0.96	0.07	22,25,30,31	0
3	A1A0J	A	502	19/19	0.96	0.07	21,25,29,30	0
4	SO4	B	503	5/5	0.97	0.06	36,37,41,43	0
4	SO4	C	504	5/5	0.97	0.07	26,26,32,32	0
3	A1A0J	B	502	19/19	0.97	0.06	23,27,35,35	0
4	SO4	D	503	5/5	0.98	0.07	27,27,31,39	0
3	A1A0J	C	502	19/19	0.98	0.05	22,25,29,30	0
4	SO4	E	503	5/5	0.99	0.04	28,29,32,34	0
2	ZN	E	501	1/1	1.00	0.01	23,23,23,23	0
4	SO4	C	503	5/5	1.00	0.03	29,33,34,39	0
2	ZN	F	501	1/1	1.00	0.02	21,21,21,21	0
2	ZN	A	501	1/1	1.00	0.02	26,26,26,26	0
2	ZN	B	501	1/1	1.00	0.01	25,25,25,25	0
2	ZN	C	501	1/1	1.00	0.01	20,20,20,20	0
2	ZN	D	501	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.

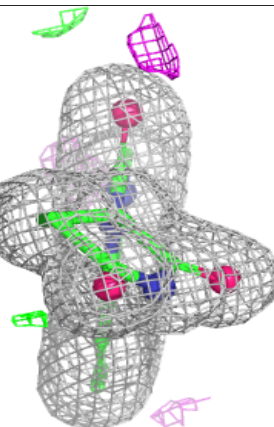
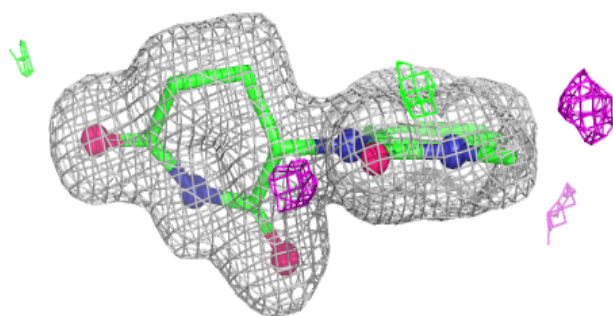
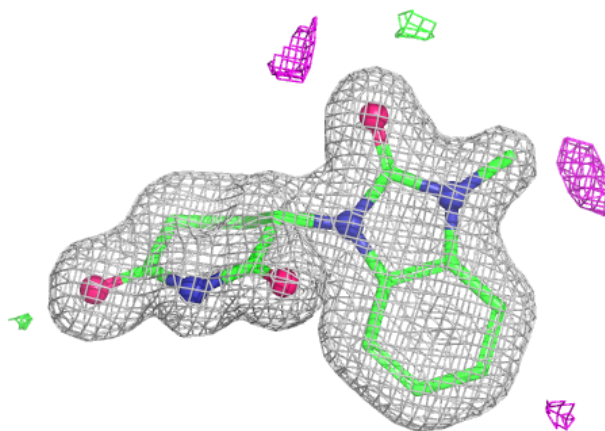
**Electron density around A1A0J E 502:**

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

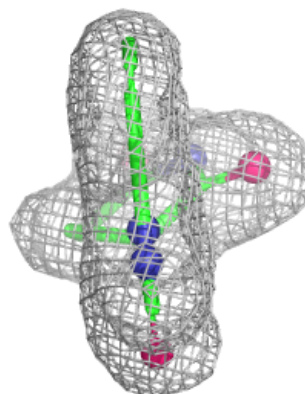
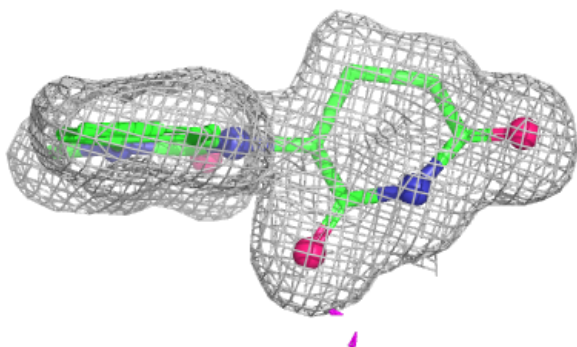
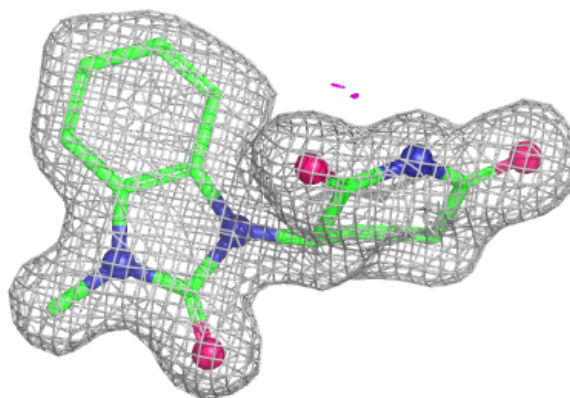


**Electron density around A1A0J F 502:**

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

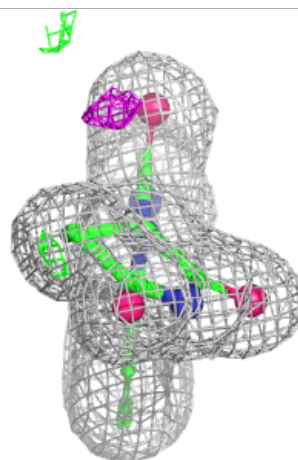
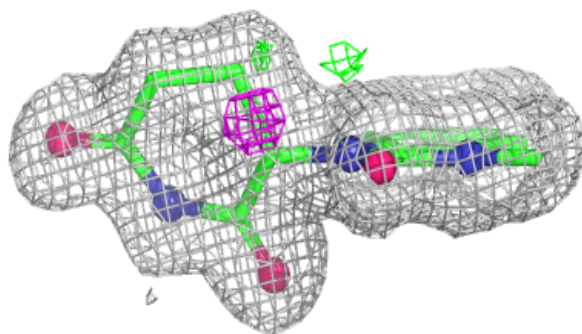
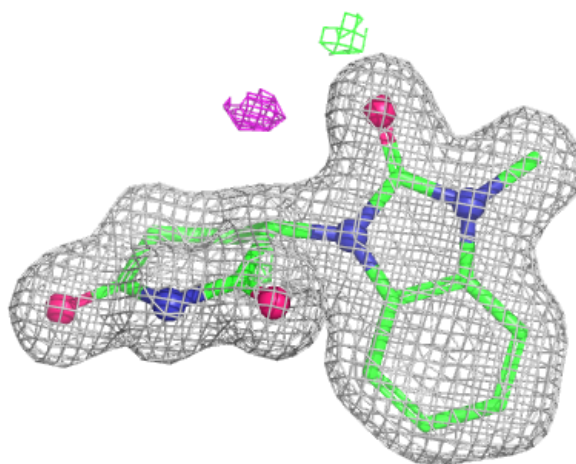
**Electron density around A1A0J D 502:**

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



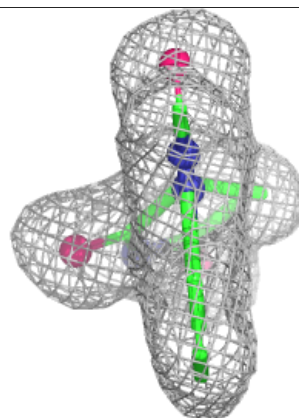
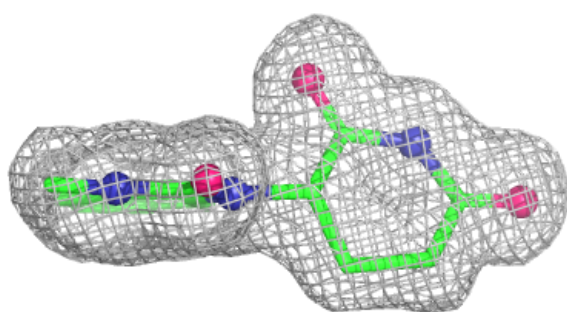
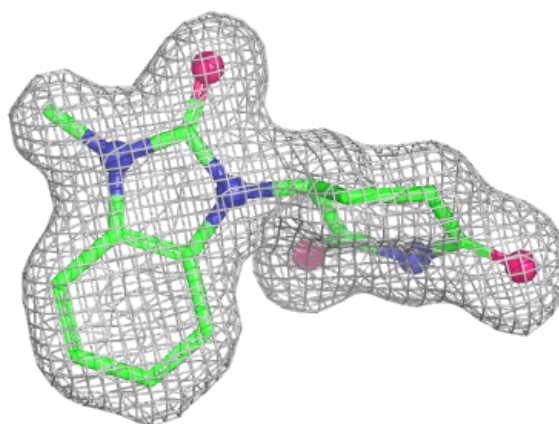
**Electron density around A1A0J A 502:**

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

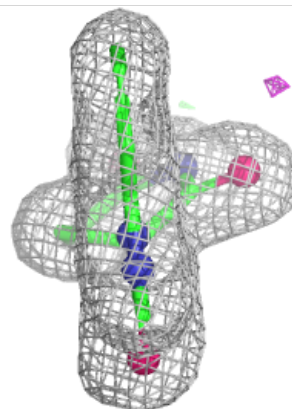
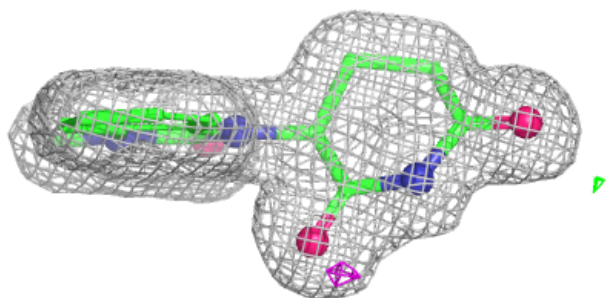
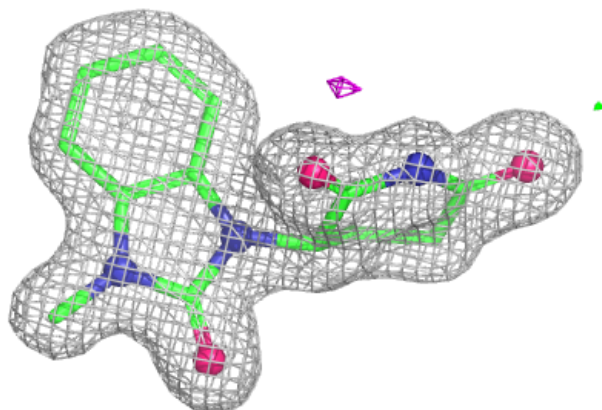


**Electron density around A1A0J B 502:**

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

**Electron density around A1A0J C 502:**

$2mF_o-DF_c$  (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.