



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 03:30 PM EDT

PDB ID : 7S76  
Title : HBV CAPSID Y132A WITH COMPOUND 10b AT 2.5Å RESOLUTION  
Authors : Olland, A.M.; Suto, R.K.  
Deposited on : 2021-09-15  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

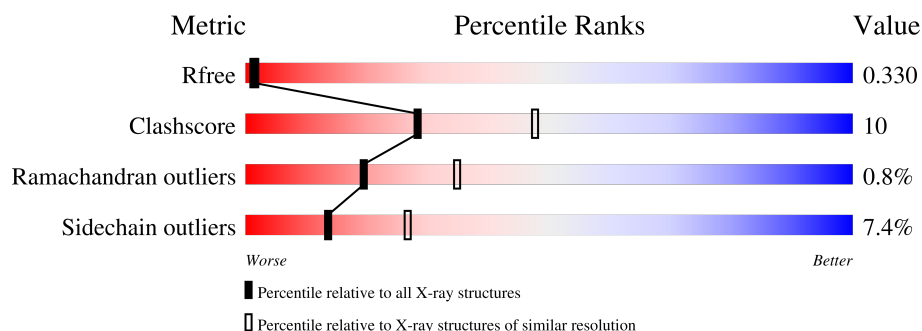
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	160	61% 23% • 14%
1	B	160	62% 22% • 14%
1	C	160	61% 19% • 17%
1	D	160	58% 23% • 17%
1	E	160	61% 21% • 17%
1	F	160	58% 20% • 21%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6466 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1086	707	179	195	5			
1	B	137	Total	C	N	O	S	0	0	0
			1077	703	178	191	5			
1	C	133	Total	C	N	O	S	0	0	0
			1045	682	173	185	5			
1	D	133	Total	C	N	O	S	0	0	0
			1040	680	170	185	5			
1	E	133	Total	C	N	O	S	0	0	0
			1034	675	170	184	5			
1	F	126	Total	C	N	O	S	0	0	0
			998	650	165	178	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP L7R9I1
A	-1	GLY	-	expression tag	UNP L7R9I1
A	0	SER	-	expression tag	UNP L7R9I1
A	132	ALA	TYR	engineered mutation	UNP L7R9I1
A	150	LYS	-	expression tag	UNP L7R9I1
A	151	LEU	-	expression tag	UNP L7R9I1
A	152	GLU	-	expression tag	UNP L7R9I1
A	153	ASN	-	expression tag	UNP L7R9I1
A	154	LEU	-	expression tag	UNP L7R9I1
A	155	TYR	-	expression tag	UNP L7R9I1
A	156	PHE	-	expression tag	UNP L7R9I1
A	157	GLN	-	expression tag	UNP L7R9I1
B	-2	MET	-	initiating methionine	UNP L7R9I1
B	-1	GLY	-	expression tag	UNP L7R9I1
B	0	SER	-	expression tag	UNP L7R9I1
B	132	ALA	TYR	engineered mutation	UNP L7R9I1
B	150	LYS	-	expression tag	UNP L7R9I1

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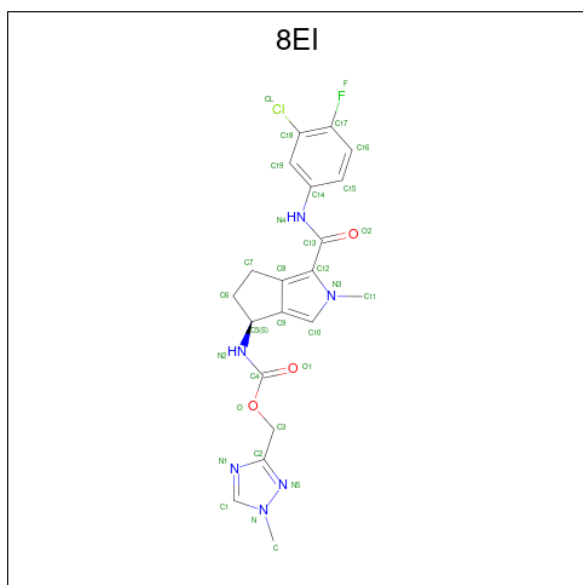
Chain	Residue	Modelled	Actual	Comment	Reference
B	151	LEU	-	expression tag	UNP L7R9I1
B	152	GLU	-	expression tag	UNP L7R9I1
B	153	ASN	-	expression tag	UNP L7R9I1
B	154	LEU	-	expression tag	UNP L7R9I1
B	155	TYR	-	expression tag	UNP L7R9I1
B	156	PHE	-	expression tag	UNP L7R9I1
B	157	GLN	-	expression tag	UNP L7R9I1
C	-2	MET	-	initiating methionine	UNP L7R9I1
C	-1	GLY	-	expression tag	UNP L7R9I1
C	0	SER	-	expression tag	UNP L7R9I1
C	132	ALA	TYR	engineered mutation	UNP L7R9I1
C	150	LYS	-	expression tag	UNP L7R9I1
C	151	LEU	-	expression tag	UNP L7R9I1
C	152	GLU	-	expression tag	UNP L7R9I1
C	153	ASN	-	expression tag	UNP L7R9I1
C	154	LEU	-	expression tag	UNP L7R9I1
C	155	TYR	-	expression tag	UNP L7R9I1
C	156	PHE	-	expression tag	UNP L7R9I1
C	157	GLN	-	expression tag	UNP L7R9I1
D	-2	MET	-	initiating methionine	UNP L7R9I1
D	-1	GLY	-	expression tag	UNP L7R9I1
D	0	SER	-	expression tag	UNP L7R9I1
D	132	ALA	TYR	engineered mutation	UNP L7R9I1
D	150	LYS	-	expression tag	UNP L7R9I1
D	151	LEU	-	expression tag	UNP L7R9I1
D	152	GLU	-	expression tag	UNP L7R9I1
D	153	ASN	-	expression tag	UNP L7R9I1
D	154	LEU	-	expression tag	UNP L7R9I1
D	155	TYR	-	expression tag	UNP L7R9I1
D	156	PHE	-	expression tag	UNP L7R9I1
D	157	GLN	-	expression tag	UNP L7R9I1
E	-2	MET	-	initiating methionine	UNP L7R9I1
E	-1	GLY	-	expression tag	UNP L7R9I1
E	0	SER	-	expression tag	UNP L7R9I1
E	132	ALA	TYR	engineered mutation	UNP L7R9I1
E	150	LYS	-	expression tag	UNP L7R9I1
E	151	LEU	-	expression tag	UNP L7R9I1
E	152	GLU	-	expression tag	UNP L7R9I1
E	153	ASN	-	expression tag	UNP L7R9I1
E	154	LEU	-	expression tag	UNP L7R9I1
E	155	TYR	-	expression tag	UNP L7R9I1
E	156	PHE	-	expression tag	UNP L7R9I1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	157	GLN	-	expression tag	UNP L7R9I1
F	-2	MET	-	initiating methionine	UNP L7R9I1
F	-1	GLY	-	expression tag	UNP L7R9I1
F	0	SER	-	expression tag	UNP L7R9I1
F	132	ALA	TYR	engineered mutation	UNP L7R9I1
F	150	LYS	-	expression tag	UNP L7R9I1
F	151	LEU	-	expression tag	UNP L7R9I1
F	152	GLU	-	expression tag	UNP L7R9I1
F	153	ASN	-	expression tag	UNP L7R9I1
F	154	LEU	-	expression tag	UNP L7R9I1
F	155	TYR	-	expression tag	UNP L7R9I1
F	156	PHE	-	expression tag	UNP L7R9I1
F	157	GLN	-	expression tag	UNP L7R9I1

- Molecule 2 is (1-methyl-1H-1,2,4-triazol-3-yl)methyl {(4S)-1-[(3-chloro-4-fluorophenyl)carbamoyl]-2-methyl-2,4,5,6-tetrahydrocyclopenta[c]pyrrol-4-yl}carbamate (three-letter code: 8EI) (formula: C<sub>20</sub>H<sub>20</sub>ClFN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		
2	C	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		
2	D	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		

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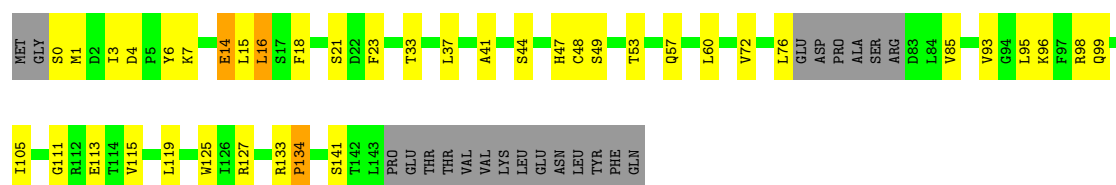
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		
2	F	1	Total	C	Cl	F	N	O	0	0
			31	20	1	1	6	3		

### 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. 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. 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.

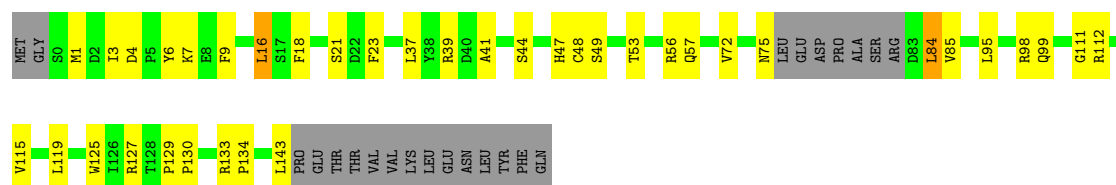
- Molecule 1: Capsid protein

Chain A: 



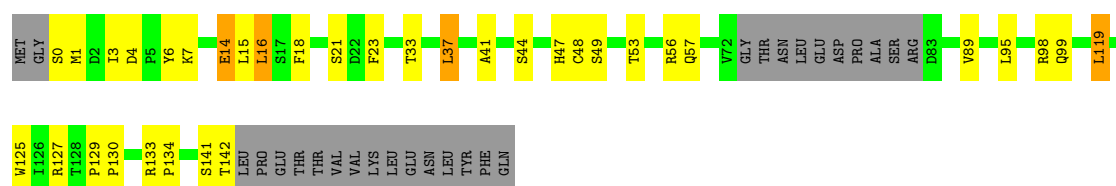
- Molecule 1: Capsid protein

Chain B: 



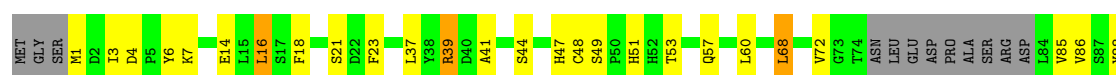
- Molecule 1: Capsid protein

Chain C: 



- Molecule 1: Capsid protein

Chain D: 





● Molecule 1: Capsid protein



● Molecule 1: Capsid protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.24Å 88.31Å 103.71Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	47.26 – 2.50 47.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.26-2.50) 99.4 (47.21-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.270 , 0.297 0.297 , 0.330	Depositor DCC
$R_{free}$ test set	2307 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.10% 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: 8EI

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	0.68	0/1118	0.75	0/1531
1	B	0.69	0/1109	0.74	0/1520
1	C	0.69	0/1077	0.75	0/1476
1	D	0.70	0/1072	0.75	0/1470
1	E	0.69	0/1065	0.75	0/1459
1	F	0.68	0/1029	0.74	0/1408
All	All	0.69	0/6470	0.74	0/8864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1086	0	1061	23	0
1	B	1077	0	1060	24	0
1	C	1045	0	1017	21	0
1	D	1040	0	1014	23	0
1	E	1034	0	1006	22	0
1	F	998	0	975	20	0
2	A	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	3	0
2	E	31	0	0	1	0
2	F	31	0	0	1	0
All	All	6466	0	6133	124	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 10.

All (124) 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:3:ILE:HG22	1:F:60:LEU:HD11	1.82	0.61
1:D:68:LEU:O	1:D:72:VAL:HG23	2.03	0.59
1:C:0:SER:O	1:D:39:ARG:NH2	2.35	0.58
1:B:4:ASP:HB3	1:B:7:LYS:HB2	1.86	0.57
1:C:4:ASP:HB3	1:C:7:LYS:HB2	1.87	0.57
1:C:53:THR:O	1:C:57:GLN:HG2	2.07	0.55
1:F:4:ASP:HB3	1:F:7:LYS:HB2	1.88	0.55
1:B:53:THR:O	1:B:57:GLN:HG2	2.07	0.54
1:A:53:THR:O	1:A:57:GLN:HG2	2.07	0.54
1:A:134:PRO:HG3	1:F:139:ILE:HG12	1.89	0.54
1:D:53:THR:O	1:D:57:GLN:HG2	2.08	0.54
1:E:4:ASP:HB3	1:E:7:LYS:HB2	1.89	0.54
1:E:53:THR:O	1:E:57:GLN:HG2	2.07	0.54
1:A:4:ASP:HB3	1:A:7:LYS:HB2	1.89	0.54
1:F:53:THR:O	1:F:57:GLN:HG2	2.07	0.54
1:A:60:LEU:HD11	1:B:3:ILE:HG22	1.89	0.54
1:C:141:SER:O	1:C:142:THR:OG1	2.24	0.54
1:D:4:ASP:HB3	1:D:7:LYS:HB2	1.88	0.53
1:B:6:TYR:CE1	1:B:16:LEU:HD13	2.44	0.52
1:E:6:TYR:CE1	1:E:16:LEU:HD13	2.45	0.52
1:A:6:TYR:CE1	1:A:16:LEU:HD13	2.46	0.51
1:F:6:TYR:CE1	1:F:16:LEU:HD13	2.46	0.51
1:C:6:TYR:CE1	1:C:16:LEU:HD13	2.46	0.50
1:A:33:THR:HG22	1:A:37:LEU:HD12	1.93	0.50
1:C:3:ILE:HG22	1:D:60:LEU:HD11	1.93	0.50
1:E:60:LEU:HD11	1:F:3:ILE:HG22	1.94	0.50
1:E:95:LEU:O	1:E:99:GLN:HG3	2.12	0.50
1:D:6:TYR:CE1	1:D:16:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:O	1:C:99:GLN:HG3	2.12	0.50
1:B:72:VAL:HG11	1:B:85:VAL:HG11	1.94	0.49
2:E:201:8EI:C15	2:E:201:8EI:O2	2.59	0.49
1:D:95:LEU:O	1:D:99:GLN:HG3	2.13	0.48
1:F:95:LEU:O	1:F:99:GLN:HG3	2.13	0.48
1:B:9:PHE:HA	1:B:112:ARG:NH2	2.28	0.48
1:A:95:LEU:O	1:A:99:GLN:HG3	2.13	0.48
1:A:14:GLU:HG3	1:A:15:LEU:N	2.29	0.48
1:B:95:LEU:O	1:B:99:GLN:HG3	2.13	0.48
1:E:64:ASP:OD2	1:F:96:LYS:NZ	2.41	0.48
1:D:85:VAL:HG13	1:D:86:VAL:N	2.30	0.47
1:C:23:PHE:C	1:C:23:PHE:CD1	2.88	0.46
1:B:23:PHE:C	1:B:23:PHE:CD1	2.89	0.46
1:E:23:PHE:CD1	1:E:23:PHE:C	2.89	0.46
2:D:201:8EI:C15	2:D:201:8EI:O2	2.60	0.46
1:F:23:PHE:C	1:F:23:PHE:CD1	2.89	0.46
2:F:201:8EI:O2	2:F:201:8EI:C15	2.63	0.45
2:D:201:8EI:O1	1:E:134:PRO:HG2	2.16	0.45
1:A:3:ILE:HG21	1:B:56:ARG:HG2	1.99	0.45
1:A:23:PHE:CD1	1:A:23:PHE:C	2.90	0.45
1:D:125:TRP:CE2	1:D:133:ARG:HD2	2.52	0.45
1:E:125:TRP:CE2	1:E:133:ARG:HD2	2.52	0.45
1:D:23:PHE:C	1:D:23:PHE:CD1	2.89	0.45
1:A:72:VAL:HG11	1:A:85:VAL:HG11	1.99	0.45
1:F:125:TRP:CE2	1:F:133:ARG:HD2	2.52	0.45
1:C:23:PHE:CD1	1:C:23:PHE:O	2.70	0.44
1:A:125:TRP:CE2	1:A:133:ARG:HD2	2.53	0.44
1:B:39:ARG:NH1	1:C:14:GLU:OE2	2.37	0.44
1:B:125:TRP:CE2	1:B:133:ARG:HD2	2.53	0.44
1:C:125:TRP:CE2	1:C:133:ARG:HD2	2.52	0.44
1:F:23:PHE:CD1	1:F:23:PHE:O	2.70	0.44
1:C:56:ARG:HG2	1:D:3:ILE:HG21	2.00	0.44
1:B:23:PHE:CD1	1:B:23:PHE:O	2.71	0.44
1:E:23:PHE:CD1	1:E:23:PHE:O	2.71	0.44
1:A:41:ALA:O	1:A:44:SER:HB3	2.19	0.43
1:C:33:THR:O	1:C:37:LEU:HB2	2.19	0.43
1:D:41:ALA:O	1:D:44:SER:HB3	2.19	0.43
1:A:23:PHE:CD1	1:A:23:PHE:O	2.72	0.43
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.84	0.43
1:B:41:ALA:O	1:B:44:SER:HB3	2.18	0.42
1:E:41:ALA:O	1:E:44:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLU:CD	1:F:39:ARG:HH12	2.19	0.42
1:A:18:PHE:CD1	1:A:127:ARG:NH1	2.88	0.42
1:D:21:SER:O	1:D:98:ARG:NH2	2.53	0.42
1:D:23:PHE:CD1	1:D:23:PHE:O	2.71	0.42
1:F:21:SER:O	1:F:98:ARG:NH2	2.52	0.42
1:C:21:SER:O	1:C:98:ARG:NH2	2.52	0.42
1:E:6:TYR:CZ	1:E:16:LEU:HD13	2.54	0.42
1:A:105:ILE:HG21	2:A:201:8EI:F	2.10	0.42
1:E:47:HIS:O	1:E:48:CYS:HB2	2.20	0.42
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.85	0.42
1:D:72:VAL:HG11	1:D:85:VAL:HG21	2.00	0.42
1:F:18:PHE:CD1	1:F:127:ARG:NH1	2.87	0.42
1:F:33:THR:O	1:F:37:LEU:HB2	2.20	0.42
1:F:6:TYR:CZ	1:F:16:LEU:HD13	2.55	0.42
1:B:18:PHE:CD1	1:B:127:ARG:NH1	2.88	0.42
1:B:112:ARG:HG3	1:B:112:ARG:HH21	1.84	0.42
1:E:16:LEU:HB3	1:E:99:GLN:OE1	2.20	0.42
1:C:18:PHE:CD1	1:C:127:ARG:NH1	2.88	0.41
1:C:15:LEU:HG	1:C:119:LEU:HD23	2.02	0.41
1:E:134:PRO:HA	1:E:135:PRO:HD3	1.94	0.41
1:C:129:PRO:HA	1:C:130:PRO:HD3	1.97	0.41
1:D:6:TYR:CZ	1:D:16:LEU:HD13	2.56	0.41
1:D:16:LEU:HB3	1:D:99:GLN:OE1	2.21	0.41
1:B:4:ASP:HB3	1:B:7:LYS:CB	2.51	0.41
1:C:6:TYR:CZ	1:C:16:LEU:HD13	2.56	0.41
1:A:4:ASP:HB3	1:A:7:LYS:CB	2.50	0.41
1:A:21:SER:O	1:A:98:ARG:NH2	2.53	0.41
1:C:47:HIS:O	1:C:48:CYS:HB2	2.20	0.41
1:E:21:SER:O	1:E:98:ARG:NH2	2.53	0.41
1:E:129:PRO:HA	1:E:130:PRO:HD3	1.96	0.41
1:F:111:GLY:O	1:F:115:VAL:HG23	2.20	0.41
1:A:111:GLY:O	1:A:115:VAL:HG23	2.21	0.41
1:B:16:LEU:HB3	1:B:99:GLN:OE1	2.20	0.41
1:B:21:SER:O	1:B:98:ARG:NH2	2.52	0.41
1:B:129:PRO:HA	1:B:130:PRO:HD3	1.98	0.41
1:F:41:ALA:O	1:F:44:SER:HB3	2.20	0.41
1:B:47:HIS:O	1:B:48:CYS:HB2	2.21	0.41
1:C:41:ALA:O	1:C:44:SER:HB3	2.19	0.41
1:F:129:PRO:HA	1:F:130:PRO:HD3	1.96	0.41
1:D:51:HIS:NE2	1:D:112:ARG:CZ	2.84	0.41
1:B:6:TYR:CZ	1:B:16:LEU:HD13	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PHE:CD1	1:D:127:ARG:NH1	2.89	0.40
1:A:23:PHE:O	1:A:23:PHE:CG	2.74	0.40
1:C:4:ASP:HB3	1:C:7:LYS:CB	2.51	0.40
1:D:111:GLY:O	1:D:115:VAL:HG23	2.21	0.40
1:A:6:TYR:CZ	1:A:16:LEU:HD13	2.56	0.40
1:D:105:ILE:HG21	2:D:201:8EI:F	2.12	0.40
1:B:9:PHE:HD1	1:B:112:ARG:HH22	1.68	0.40
1:E:18:PHE:CD1	1:E:127:ARG:NH1	2.90	0.40
1:E:111:GLY:O	1:E:115:VAL:HG23	2.21	0.40
1:A:47:HIS:O	1:A:48:CYS:HB2	2.21	0.40
1:B:111:GLY:O	1:B:115:VAL:HG23	2.21	0.40
1:D:47:HIS:O	1:D:48:CYS:HB2	2.21	0.40
1:D:139:ILE:HG12	1:E:134:PRO:HG3	2.04	0.40
1:F:4:ASP:HB3	1:F:7:LYS:CB	2.51	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	134/160 (84%)	123 (92%)	10 (8%)	1 (1%)	22	39
1	B	133/160 (83%)	124 (93%)	8 (6%)	1 (1%)	19	35
1	C	129/160 (81%)	120 (93%)	8 (6%)	1 (1%)	19	35
1	D	129/160 (81%)	118 (92%)	10 (8%)	1 (1%)	19	35
1	E	129/160 (81%)	118 (92%)	10 (8%)	1 (1%)	19	35
1	F	122/160 (76%)	113 (93%)	8 (7%)	1 (1%)	19	35
All	All	776/960 (81%)	716 (92%)	54 (7%)	6 (1%)	19	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	134	PRO
1	A	134	PRO
1	D	134	PRO
1	E	134	PRO
1	C	134	PRO
1	B	134	PRO

### 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	118/141 (84%)	107 (91%)	11 (9%)	9	17
1	B	117/141 (83%)	109 (93%)	8 (7%)	16	30
1	C	112/141 (79%)	105 (94%)	7 (6%)	18	34
1	D	112/141 (79%)	102 (91%)	10 (9%)	9	19
1	E	110/141 (78%)	103 (94%)	7 (6%)	17	33
1	F	108/141 (77%)	101 (94%)	7 (6%)	17	33
All	All	677/846 (80%)	627 (93%)	50 (7%)	13	27

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	1	MET
1	A	14	GLU
1	A	16	LEU
1	A	49	SER
1	A	76	LEU
1	A	93	VAL
1	A	96	LYS
1	A	113	GLU
1	A	119	LEU
1	A	141	SER
1	B	1	MET
1	B	16	LEU

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Mol	Chain	Res	Type
1	B	37	LEU
1	B	49	SER
1	B	75	ASN
1	B	84	LEU
1	B	119	LEU
1	B	143	LEU
1	C	1	MET
1	C	14	GLU
1	C	16	LEU
1	C	37	LEU
1	C	49	SER
1	C	89	VAL
1	C	119	LEU
1	D	1	MET
1	D	14	GLU
1	D	16	LEU
1	D	37	LEU
1	D	39	ARG
1	D	49	SER
1	D	68	LEU
1	D	88	TYR
1	D	93	VAL
1	D	119	LEU
1	E	0	SER
1	E	1	MET
1	E	16	LEU
1	E	37	LEU
1	E	49	SER
1	E	93	VAL
1	E	119	LEU
1	F	1	MET
1	F	16	LEU
1	F	37	LEU
1	F	45	PRO
1	F	49	SER
1	F	93	VAL
1	F	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	8EI	D	201	-	27,34,34	2.19	6 (22%)	31,49,49	2.20	10 (32%)
2	8EI	E	201	-	27,34,34	2.04	6 (22%)	31,49,49	2.02	12 (38%)
2	8EI	A	201	-	27,34,34	2.09	7 (25%)	31,49,49	1.87	7 (22%)
2	8EI	C	201	-	27,34,34	1.97	6 (22%)	31,49,49	2.05	10 (32%)
2	8EI	F	201	-	27,34,34	2.12	6 (22%)	31,49,49	2.00	8 (25%)
2	8EI	B	201	-	27,34,34	2.09	6 (22%)	31,49,49	1.92	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8EI	D	201	-	-	7/11/26/26	0/4/4/4
2	8EI	E	201	-	-	4/11/26/26	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8EI	A	201	-	-	4/11/26/26	0/4/4/4
2	8EI	C	201	-	-	6/11/26/26	0/4/4/4
2	8EI	F	201	-	-	5/11/26/26	0/4/4/4
2	8EI	B	201	-	-	4/11/26/26	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	8EI	C18-C17	6.32	1.47	1.38
2	B	201	8EI	C18-C17	6.06	1.47	1.38
2	A	201	8EI	O-C4	6.00	1.46	1.35
2	F	201	8EI	O-C4	5.79	1.46	1.35
2	E	201	8EI	O-C4	5.73	1.46	1.35
2	D	201	8EI	O-C4	5.71	1.46	1.35
2	F	201	8EI	C18-C17	5.63	1.46	1.38
2	A	201	8EI	C18-C17	5.57	1.46	1.38
2	C	201	8EI	C18-C17	5.43	1.46	1.38
2	C	201	8EI	O-C4	5.20	1.45	1.35
2	E	201	8EI	C18-C17	5.07	1.45	1.38
2	B	201	8EI	O-C4	4.95	1.44	1.35
2	D	201	8EI	C9-C5	-4.53	1.45	1.51
2	E	201	8EI	C9-C5	-4.52	1.45	1.51
2	B	201	8EI	C9-C5	-4.49	1.45	1.51
2	F	201	8EI	C9-C5	-4.39	1.45	1.51
2	C	201	8EI	C9-C5	-4.10	1.46	1.51
2	A	201	8EI	C9-C5	-4.06	1.46	1.51
2	D	201	8EI	C14-N4	-2.89	1.35	1.41
2	E	201	8EI	C14-N4	-2.76	1.36	1.41
2	F	201	8EI	C14-N4	-2.73	1.36	1.41
2	B	201	8EI	C18-CL	2.71	1.80	1.73
2	A	201	8EI	C12-C8	2.67	1.47	1.40
2	B	201	8EI	C14-N4	-2.60	1.36	1.41
2	F	201	8EI	C12-C8	2.57	1.47	1.40
2	D	201	8EI	C12-C8	2.50	1.47	1.40
2	C	201	8EI	C12-C8	2.48	1.47	1.40
2	A	201	8EI	C14-N4	-2.45	1.36	1.41
2	D	201	8EI	C18-CL	2.39	1.79	1.73
2	B	201	8EI	C12-C8	2.36	1.47	1.40
2	C	201	8EI	C14-N4	-2.33	1.36	1.41
2	F	201	8EI	C18-CL	2.31	1.79	1.73
2	E	201	8EI	C12-C8	2.22	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	8EI	C18-CL	2.22	1.78	1.73
2	E	201	8EI	C18-CL	2.16	1.78	1.73
2	A	201	8EI	C18-CL	2.12	1.78	1.73
2	A	201	8EI	C8-C9	2.02	1.41	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	8EI	C-N-N5	-5.31	114.27	120.50
2	B	201	8EI	C-N-N5	-5.20	114.39	120.50
2	F	201	8EI	C7-C6-C5	5.01	113.59	105.54
2	E	201	8EI	C7-C6-C5	5.00	113.57	105.54
2	C	201	8EI	C7-C6-C5	4.90	113.42	105.54
2	C	201	8EI	C-N-N5	-4.83	114.83	120.50
2	A	201	8EI	C7-C6-C5	4.73	113.14	105.54
2	B	201	8EI	C7-C6-C5	4.57	112.88	105.54
2	D	201	8EI	C7-C6-C5	4.56	112.87	105.54
2	F	201	8EI	C-N-N5	-4.50	115.22	120.50
2	D	201	8EI	C6-C5-N2	-3.90	106.64	114.59
2	A	201	8EI	C-N-N5	-3.90	115.92	120.50
2	D	201	8EI	C6-C7-C8	-3.85	99.36	103.30
2	E	201	8EI	C-N-N5	-3.78	116.07	120.50
2	E	201	8EI	C6-C7-C8	-3.71	99.50	103.30
2	A	201	8EI	C3-O-C4	3.68	124.14	115.93
2	E	201	8EI	O-C4-N2	3.61	117.84	110.50
2	F	201	8EI	C6-C7-C8	-3.56	99.65	103.30
2	C	201	8EI	C6-C7-C8	-3.46	99.76	103.30
2	B	201	8EI	C10-N3-C12	3.45	112.36	108.66
2	F	201	8EI	C16-C17-C18	-3.41	118.23	121.32
2	B	201	8EI	C6-C7-C8	-3.39	99.82	103.30
2	D	201	8EI	C3-O-C4	3.39	123.50	115.93
2	C	201	8EI	O-C4-N2	3.27	117.15	110.50
2	F	201	8EI	C3-O-C4	3.24	123.17	115.93
2	D	201	8EI	C5-N2-C4	-3.19	117.83	121.93
2	A	201	8EI	C6-C7-C8	-3.06	100.16	103.30
2	C	201	8EI	C10-N3-C12	3.03	111.91	108.66
2	D	201	8EI	C10-N3-C12	3.02	111.89	108.66
2	F	201	8EI	C6-C5-N2	-2.98	108.52	114.59
2	D	201	8EI	O-C4-N2	2.95	116.49	110.50
2	A	201	8EI	C10-N3-C12	2.88	111.75	108.66
2	A	201	8EI	C16-C17-C18	-2.82	118.77	121.32
2	F	201	8EI	C10-N3-C12	2.74	111.59	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	8EI	C6-C5-N2	-2.73	109.02	114.59
2	E	201	8EI	C19-C18-CL	2.71	122.86	118.49
2	E	201	8EI	C10-N3-C12	2.69	111.54	108.66
2	D	201	8EI	C16-C17-C18	-2.57	119.00	121.32
2	C	201	8EI	O-C4-O1	-2.54	119.37	124.25
2	E	201	8EI	C6-C5-N2	-2.47	109.55	114.59
2	C	201	8EI	C16-C17-C18	-2.44	119.12	121.32
2	C	201	8EI	C19-C18-CL	2.42	122.40	118.49
2	B	201	8EI	C16-C17-C18	-2.35	119.19	121.32
2	D	201	8EI	O-C4-O1	-2.30	119.83	124.25
2	C	201	8EI	F-C17-C16	2.29	123.71	118.59
2	C	201	8EI	C3-O-C4	2.28	121.02	115.93
2	E	201	8EI	F-C17-C16	2.22	123.55	118.59
2	E	201	8EI	O1-C4-N2	-2.18	121.28	124.85
2	E	201	8EI	C16-C17-C18	-2.17	119.35	121.32
2	F	201	8EI	F-C17-C16	2.11	123.30	118.59
2	E	201	8EI	C17-C18-CL	-2.09	117.25	119.78
2	E	201	8EI	F-C17-C18	-2.05	117.08	118.98
2	B	201	8EI	C6-C5-N2	-2.02	110.48	114.59

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	8EI	C12-C13-N4-C14
2	B	201	8EI	C9-C5-N2-C4
2	D	201	8EI	O1-C4-O-C3
2	D	201	8EI	N2-C4-O-C3
2	D	201	8EI	O-C4-N2-C5
2	E	201	8EI	N2-C4-O-C3
2	C	201	8EI	N2-C4-O-C3
2	E	201	8EI	O1-C4-O-C3
2	A	201	8EI	N2-C4-O-C3
2	D	201	8EI	C12-C13-N4-C14
2	C	201	8EI	C12-C13-N4-C14
2	B	201	8EI	N2-C4-O-C3
2	C	201	8EI	O1-C4-O-C3
2	F	201	8EI	C12-C13-N4-C14
2	F	201	8EI	O-C4-N2-C5
2	F	201	8EI	N2-C4-O-C3
2	A	201	8EI	O1-C4-O-C3
2	D	201	8EI	O1-C4-N2-C5

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Mol	Chain	Res	Type	Atoms
2	B	201	8EI	O-C4-N2-C5
2	C	201	8EI	C9-C5-N2-C4
2	D	201	8EI	C9-C5-N2-C4
2	E	201	8EI	C9-C5-N2-C4
2	F	201	8EI	C9-C5-N2-C4
2	C	201	8EI	C6-C5-N2-C4
2	D	201	8EI	C6-C5-N2-C4
2	E	201	8EI	C6-C5-N2-C4
2	B	201	8EI	O1-C4-O-C3
2	F	201	8EI	O1-C4-O-C3
2	C	201	8EI	C2-C3-O-C4
2	A	201	8EI	O2-C13-N4-C14

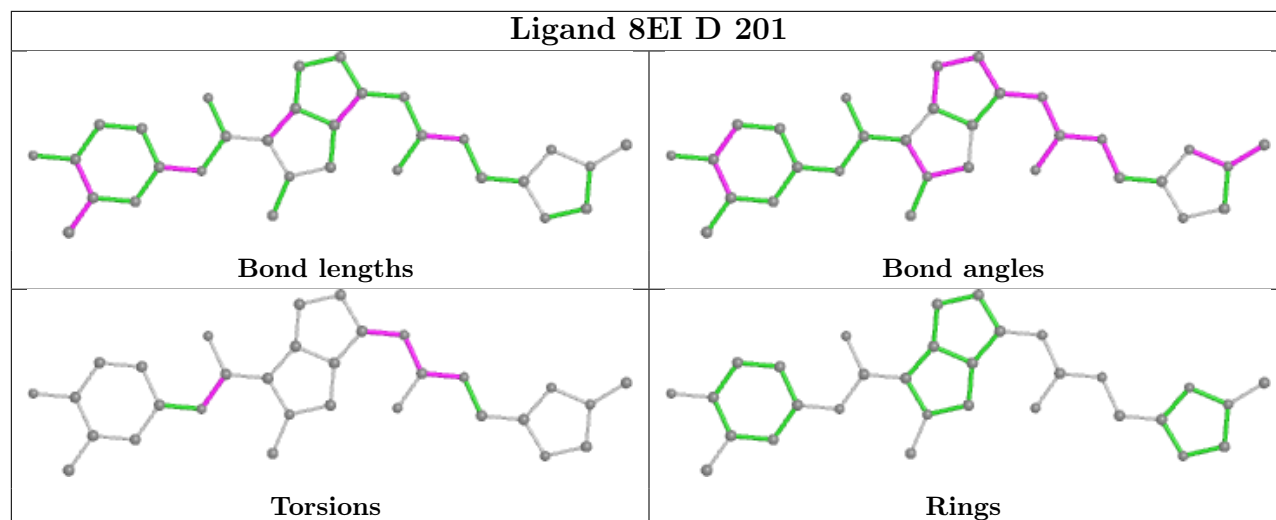
There are no ring outliers.

4 monomers are involved in 6 short contacts:

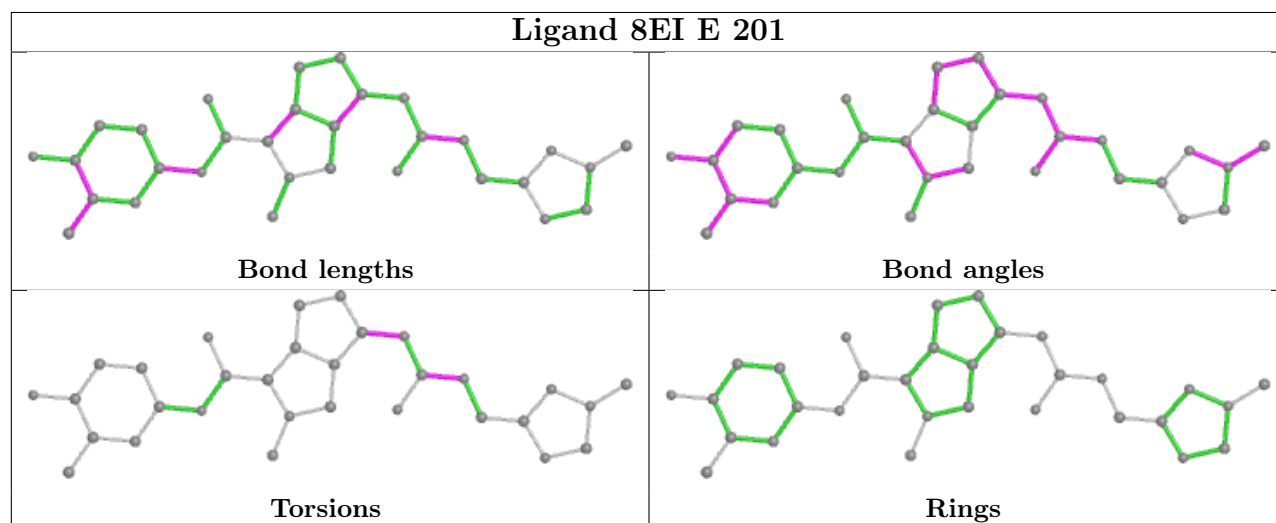
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	8EI	3	0
2	E	201	8EI	1	0
2	A	201	8EI	1	0
2	F	201	8EI	1	0

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.

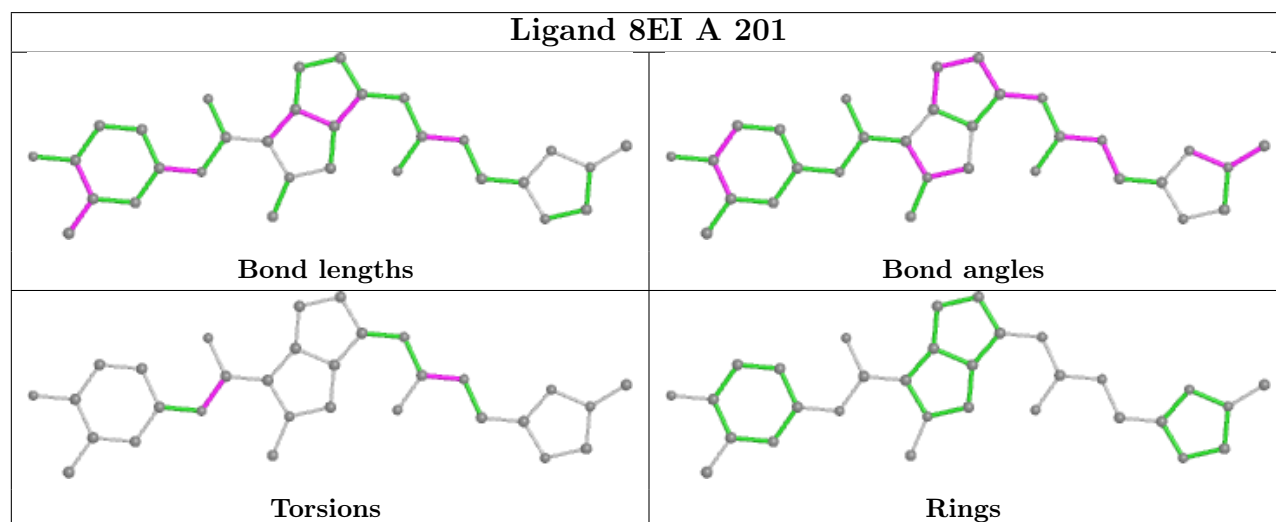
## Ligand 8EI D 201

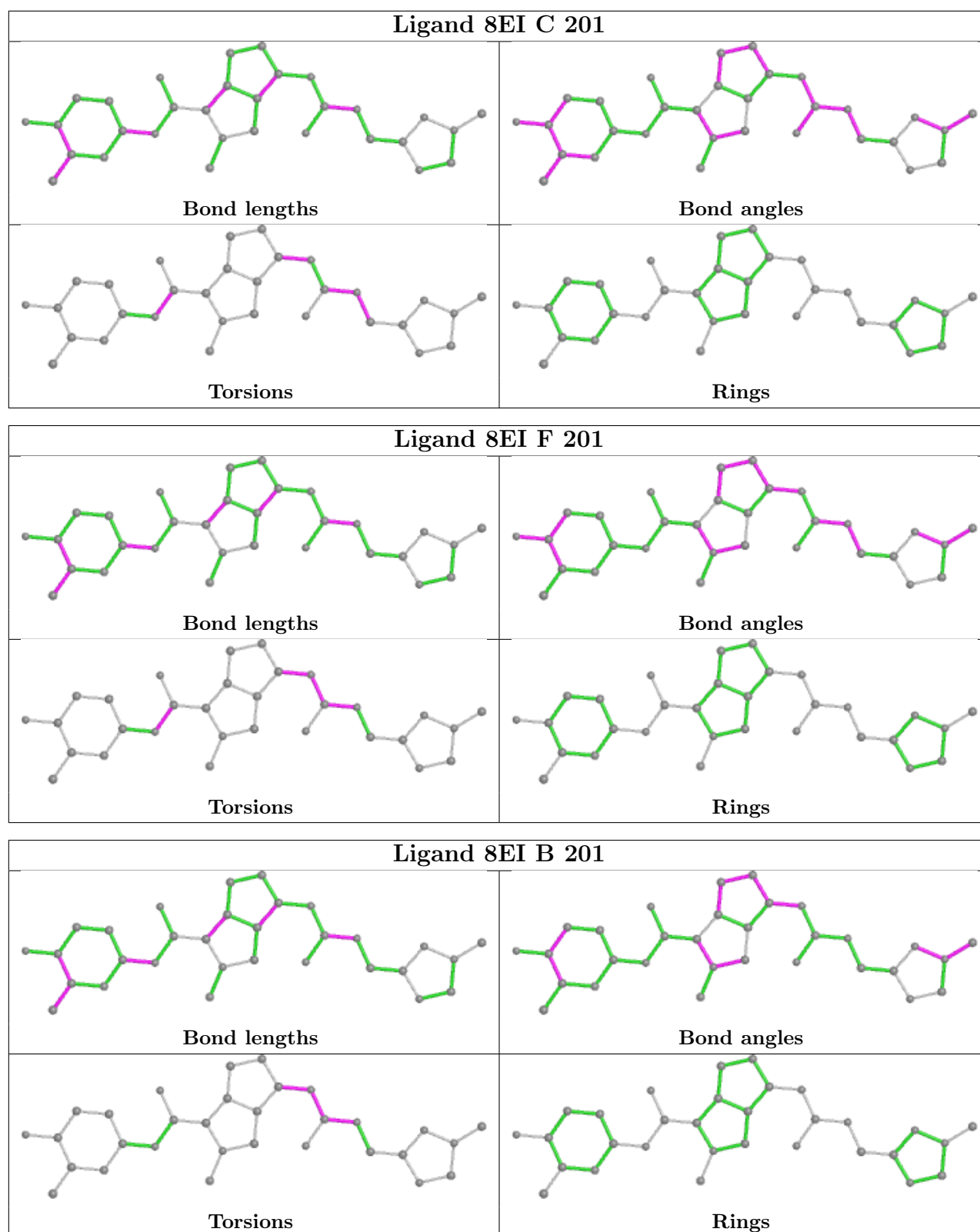


## Ligand 8EI E 201



## Ligand 8EI A 201





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

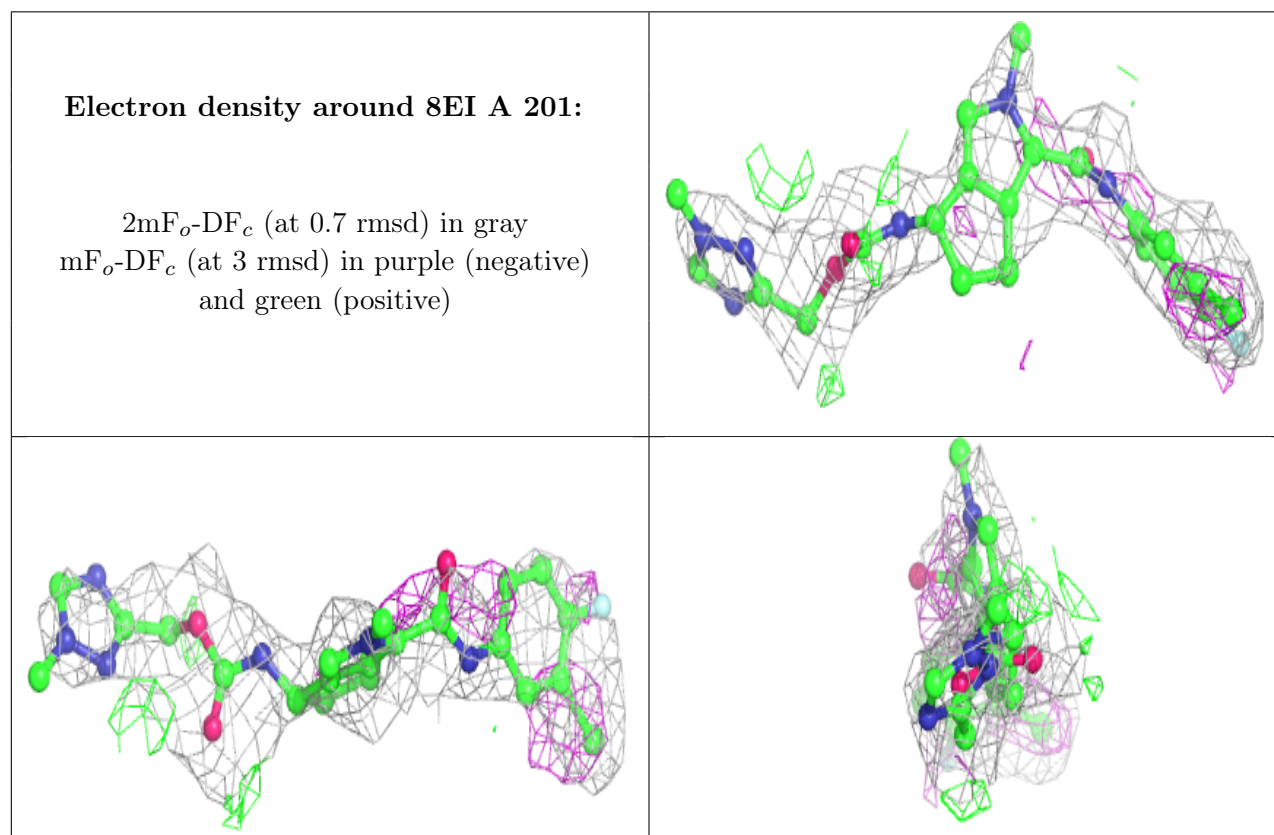
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

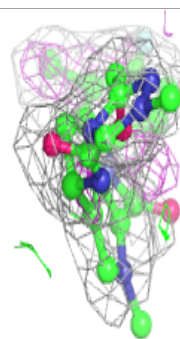
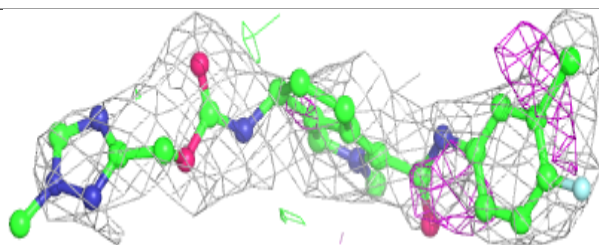
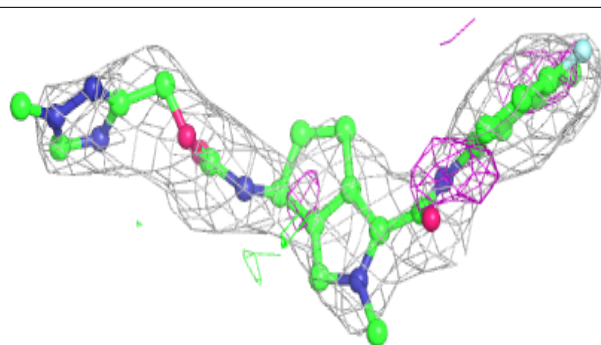
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

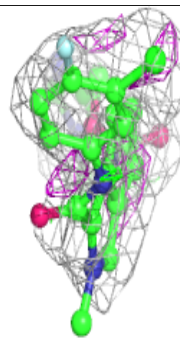
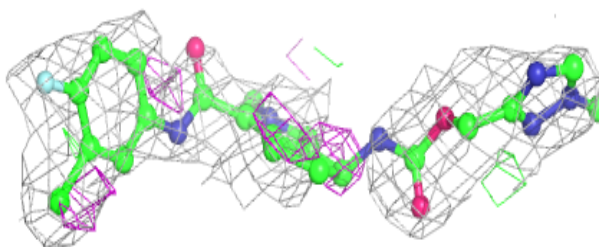
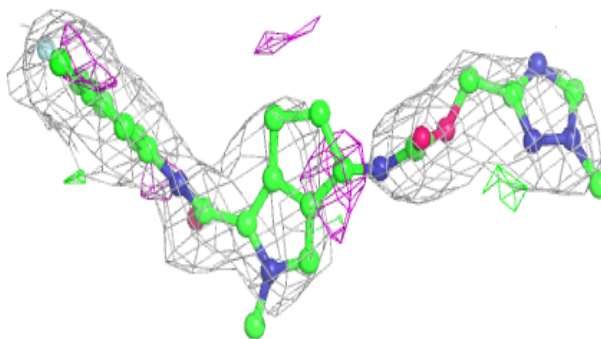


**Electron density around 8EI B 201:**

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

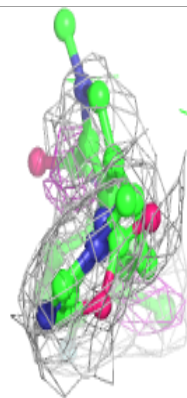
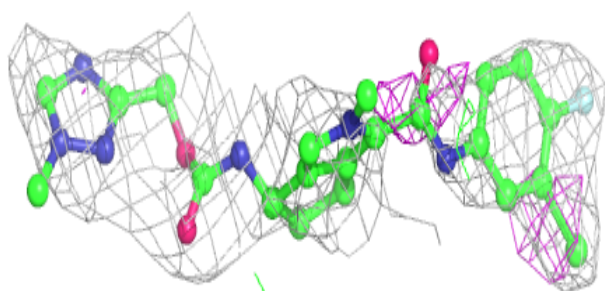
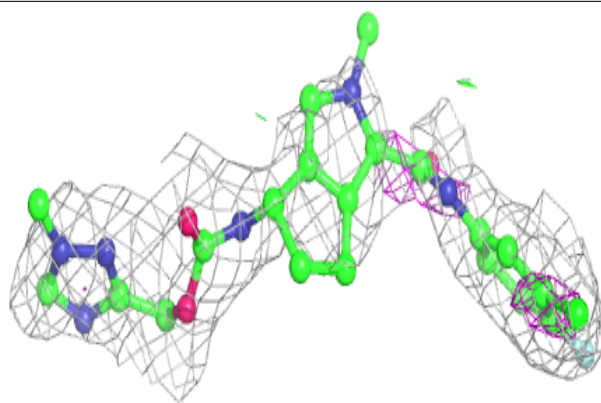
**Electron density around 8EI C 201:**

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

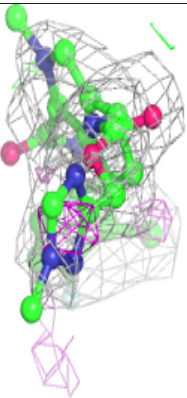
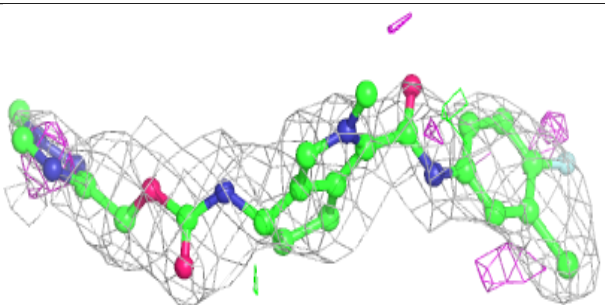
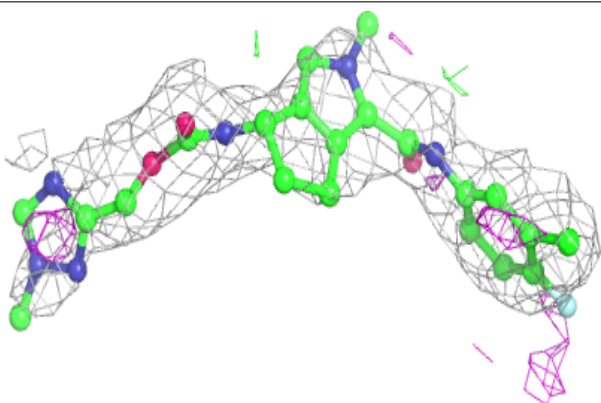


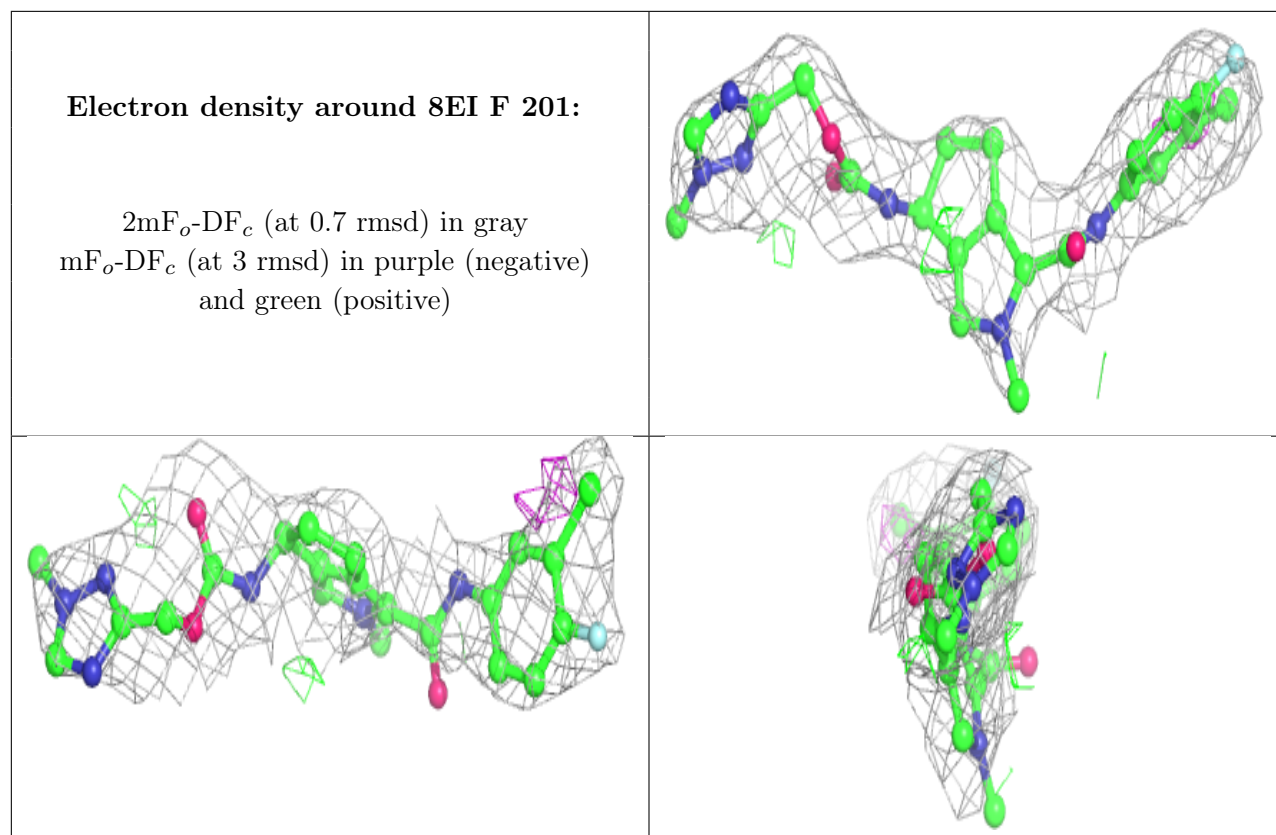
**Electron density around 8EI D 201:**

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

**Electron density around 8EI E 201:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.