



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 08:20 am BST

PDB ID : 4X4U  
Title : Crystal structure of the *A. fulgidus* CCA-adding enzyme in complex with a human MenBeta minihelix ending in CCACC  
Authors : Kuhn, C.-D.; Joshua-Tor, L.  
Deposited on : 2014-12-03  
Resolution : 2.70 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 : 2.11  
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) : 2.11

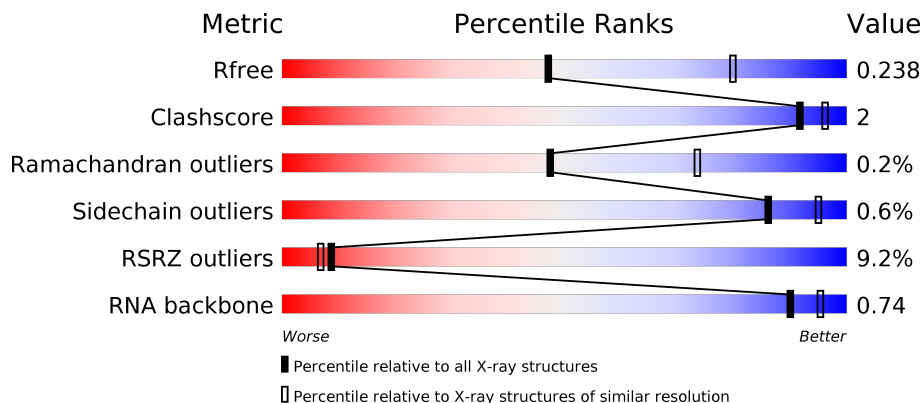
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



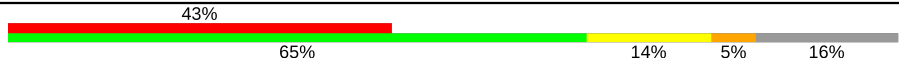

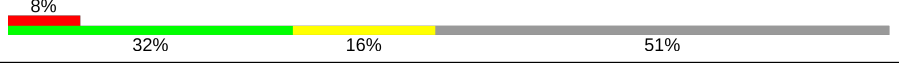
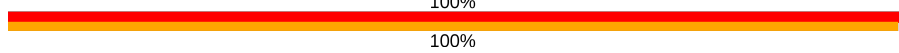
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 on 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	457	 8% 91% 5%
1	C	457	 13% 91% 5%
1	E	457	 4% 93% 5%
1	F	457	 3% 92% 5%

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Mol	Chain	Length	Quality of chain
2	B	37	
2	D	37	
2	G	37	
3	H	2	

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	APC	A	501	-	-	-	X
4	APC	F	501	-	-	-	X
5	GOL	A	503	-	-	-	X
5	GOL	A	504	-	-	-	X
5	GOL	H	101	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 31814 atoms, of which 15468 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 CCA-adding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	435	7244	2325	3629	630	647	13	0	0	0
1	C	437	7265	2333	3637	631	651	13	0	0	0
1	E	437	7285	2338	3649	634	651	13	0	1	0
1	F	436	7250	2328	3629	631	650	12	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP O28126
A	439	ASN	-	expression tag	UNP O28126
A	440	SER	-	expression tag	UNP O28126
A	441	SER	-	expression tag	UNP O28126
A	442	SER	-	expression tag	UNP O28126
A	443	VAL	-	expression tag	UNP O28126
A	444	ASP	-	expression tag	UNP O28126
A	445	LYS	-	expression tag	UNP O28126
A	446	LEU	-	expression tag	UNP O28126
A	447	ALA	-	expression tag	UNP O28126
A	448	ALA	-	expression tag	UNP O28126
A	449	ALA	-	expression tag	UNP O28126
A	450	LEU	-	expression tag	UNP O28126
A	451	GLU	-	expression tag	UNP O28126
A	452	HIS	-	expression tag	UNP O28126
A	453	HIS	-	expression tag	UNP O28126
A	454	HIS	-	expression tag	UNP O28126
A	455	HIS	-	expression tag	UNP O28126
A	456	HIS	-	expression tag	UNP O28126
A	457	HIS	-	expression tag	UNP O28126
C	438	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
C	439	ASN	-	expression tag	UNP O28126
C	440	SER	-	expression tag	UNP O28126
C	441	SER	-	expression tag	UNP O28126
C	442	SER	-	expression tag	UNP O28126
C	443	VAL	-	expression tag	UNP O28126
C	444	ASP	-	expression tag	UNP O28126
C	445	LYS	-	expression tag	UNP O28126
C	446	LEU	-	expression tag	UNP O28126
C	447	ALA	-	expression tag	UNP O28126
C	448	ALA	-	expression tag	UNP O28126
C	449	ALA	-	expression tag	UNP O28126
C	450	LEU	-	expression tag	UNP O28126
C	451	GLU	-	expression tag	UNP O28126
C	452	HIS	-	expression tag	UNP O28126
C	453	HIS	-	expression tag	UNP O28126
C	454	HIS	-	expression tag	UNP O28126
C	455	HIS	-	expression tag	UNP O28126
C	456	HIS	-	expression tag	UNP O28126
C	457	HIS	-	expression tag	UNP O28126
E	438	SER	-	expression tag	UNP O28126
E	439	ASN	-	expression tag	UNP O28126
E	440	SER	-	expression tag	UNP O28126
E	441	SER	-	expression tag	UNP O28126
E	442	SER	-	expression tag	UNP O28126
E	443	VAL	-	expression tag	UNP O28126
E	444	ASP	-	expression tag	UNP O28126
E	445	LYS	-	expression tag	UNP O28126
E	446	LEU	-	expression tag	UNP O28126
E	447	ALA	-	expression tag	UNP O28126
E	448	ALA	-	expression tag	UNP O28126
E	449	ALA	-	expression tag	UNP O28126
E	450	LEU	-	expression tag	UNP O28126
E	451	GLU	-	expression tag	UNP O28126
E	452	HIS	-	expression tag	UNP O28126
E	453	HIS	-	expression tag	UNP O28126
E	454	HIS	-	expression tag	UNP O28126
E	455	HIS	-	expression tag	UNP O28126
E	456	HIS	-	expression tag	UNP O28126
E	457	HIS	-	expression tag	UNP O28126
F	438	SER	-	expression tag	UNP O28126
F	439	ASN	-	expression tag	UNP O28126
F	440	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
F	441	SER	-	expression tag	UNP O28126
F	442	SER	-	expression tag	UNP O28126
F	443	VAL	-	expression tag	UNP O28126
F	444	ASP	-	expression tag	UNP O28126
F	445	LYS	-	expression tag	UNP O28126
F	446	LEU	-	expression tag	UNP O28126
F	447	ALA	-	expression tag	UNP O28126
F	448	ALA	-	expression tag	UNP O28126
F	449	ALA	-	expression tag	UNP O28126
F	450	LEU	-	expression tag	UNP O28126
F	451	GLU	-	expression tag	UNP O28126
F	452	HIS	-	expression tag	UNP O28126
F	453	HIS	-	expression tag	UNP O28126
F	454	HIS	-	expression tag	UNP O28126
F	455	HIS	-	expression tag	UNP O28126
F	456	HIS	-	expression tag	UNP O28126
F	457	HIS	-	expression tag	UNP O28126

- Molecule 2 is a RNA chain called human MenBeta minihelix.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	31	997	293	336	116	221	31	0	0	0
2	D	26	836	245	282	96	187	26	0	0	0
2	G	18	577	171	194	68	127	17	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-D(\*GP\*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
3	H	2	67	20	24	10	12	1	0	0	0

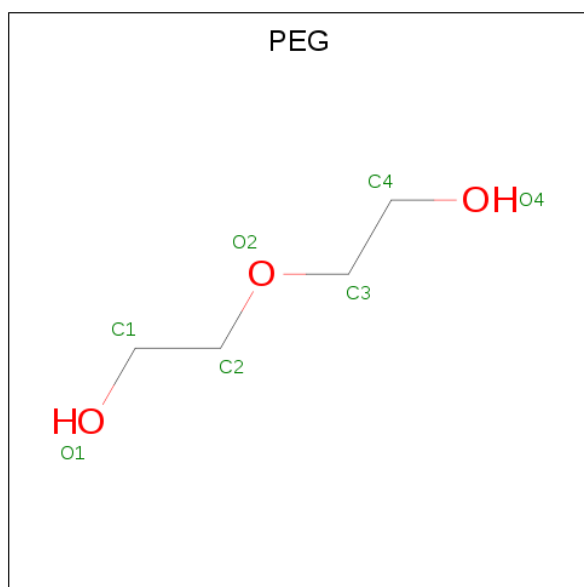
- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	E	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	26	Total	O	0	0
			26	26		
7	B	1	Total	O	0	0
			1	1		
7	C	12	Total	O	0	0
			12	12		
7	E	29	Total	O	0	0
			29	29		

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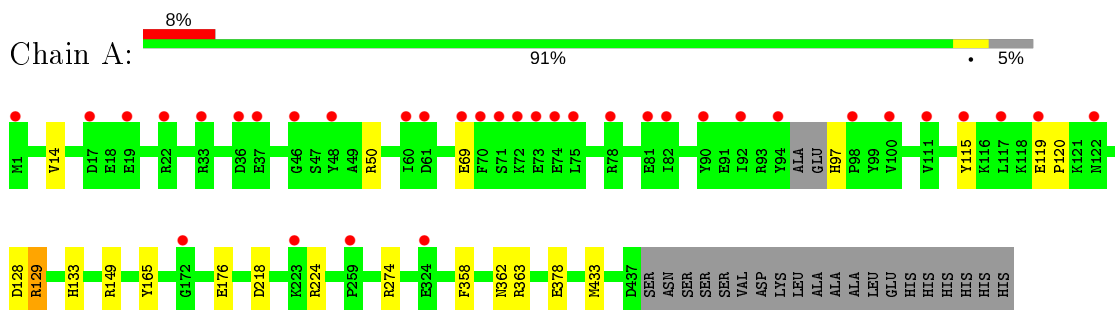
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	F	28	Total	O	0	0
			28	28		
7	G	3	Total	O	0	0
			3	3		

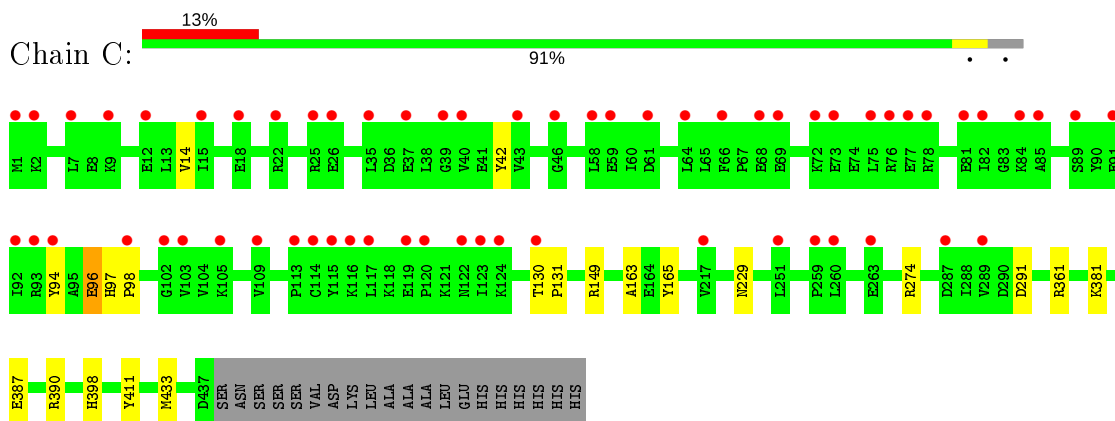
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

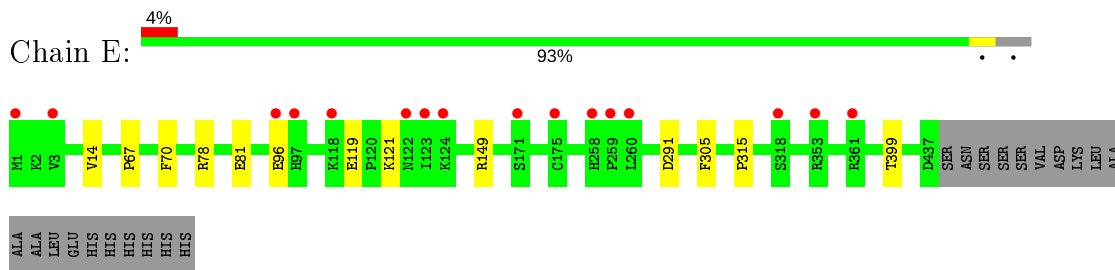
- Molecule 1: CCA-adding enzyme



- Molecule 1: CCA-adding enzyme



- Molecule 1: CCA-adding enzyme



- Molecule 1: CCA-adding enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.99Å 84.05Å 135.52Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	29.79 – 2.70 29.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.79-2.70) 97.9 (29.79-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.183 , 0.233 0.188 , 0.238	Depositor DCC
$R_{free}$ test set	3411 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, APC

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	0.31	0/3697	0.44	0/4965
1	C	0.29	0/3711	0.42	0/4985
1	E	0.34	0/3723	0.45	0/5002
1	F	0.33	0/3704	0.45	0/4977
2	B	0.44	1/735 (0.1%)	0.72	1/1140 (0.1%)
2	D	0.48	1/614 (0.2%)	0.72	1/949 (0.1%)
2	G	0.33	0/426	0.86	0/661
3	H	0.47	0/48	1.24	1/74 (1.4%)
All	All	0.33	2/16658 (0.0%)	0.49	3/22753 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.56	1.48	1.61
2	D	1	G	OP3-P	-10.55	1.48	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	G	OP1-P-O3'	5.21	116.66	105.20
3	H	1	G	OP1-P-O3'	5.13	116.48	105.20
2	B	1	G	OP1-P-O3'	5.08	116.36	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3615	3629	3621	12	0
1	C	3628	3637	3629	12	0
1	E	3636	3649	3640	6	0
1	F	3621	3629	3621	10	0
2	B	661	336	338	6	0
2	D	554	282	285	5	0
2	G	383	194	197	3	0
3	H	43	24	24	2	0
4	A	31	14	14	1	0
4	F	31	14	14	4	0
5	A	18	24	24	0	0
5	E	6	8	8	0	0
5	H	6	8	8	1	0
6	C	7	10	9	2	0
6	E	7	10	9	0	0
7	A	26	0	0	0	0
7	B	1	0	0	0	0
7	C	12	0	0	0	0
7	E	29	0	0	0	0
7	F	28	0	0	1	0
7	G	3	0	0	1	0
All	All	16346	15468	15441	50	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 2.

All (50) 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:F:299:ARG:NH1	1:F:399:THR:O	2.17	0.78
1:A:363:ARG:NH1	1:A:378:GLU:OE2	2.19	0.76
1:F:173:TYR:N	4:F:501:APC:O2A	2.18	0.74
2:B:34:C:OP2	2:B:37:C:N4	2.21	0.73
1:C:361:ARG:NH1	2:D:15:C:OP1	2.24	0.71
2:B:34:C:H3'	2:B:35:A:H5''	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH2	1:A:433:MET:O	2.27	0.68
2:B:17:A:O2'	2:B:19:U:OP2	2.17	0.62
1:E:291:ASP:OD1	2:G:31:U:O2'	2.20	0.60
1:C:387:GLU:OE2	1:C:390:ARG:NH1	2.36	0.58
1:E:119:GLU:OE1	1:E:121:LYS:NZ	2.35	0.58
2:G:25:C:OP2	7:G:103:HOH:O	2.17	0.58
1:C:274:ARG:NH2	1:C:433:MET:O	2.36	0.58
1:F:78:ARG:NH1	1:F:81:GLU:OE1	2.36	0.58
1:A:69:GLU:N	1:A:69:GLU:OE2	2.40	0.54
1:A:133:HIS:CE1	4:A:501:APC:H2	2.43	0.53
1:E:78:ARG:NH1	1:E:81:GLU:OE1	2.40	0.53
2:D:4:G:H1	2:D:31:U:H3	1.57	0.52
1:E:14:VAL:CG1	1:E:149:ARG:HB3	2.41	0.51
1:A:14:VAL:CG1	1:A:149:ARG:HB3	2.41	0.50
1:C:291:ASP:OD2	2:D:34:C:O2'	2.30	0.49
1:A:358:PHE:O	1:A:363:ARG:NH2	2.45	0.49
1:F:172:GLY:N	4:F:501:APC:O2A	2.46	0.48
1:F:163:ALA:N	4:F:501:APC:O3G	2.41	0.48
1:C:163:ALA:O	1:C:229:ASN:ND2	2.47	0.47
2:G:2:G:H1	2:G:30:U:H3	1.62	0.47
1:A:165:TYR:CE2	2:B:34:C:H1'	2.49	0.47
1:C:97:HIS:HB3	1:C:98:PRO:HD2	1.96	0.47
1:A:50:ARG:NH1	1:A:176:GLU:OE2	2.49	0.46
1:A:129:ARG:HH11	1:A:224:ARG:HD2	1.81	0.46
1:F:95:ALA:O	1:F:97:HIS:N	2.48	0.46
1:C:381:LYS:H	6:C:501:PEG:H41	1.80	0.46
1:F:172:GLY:N	4:F:501:APC:O1B	2.34	0.46
1:A:133:HIS:NE2	1:A:218:ASP:OD2	2.45	0.45
1:A:119:GLU:HB3	1:A:120:PRO:HD2	1.98	0.45
3:H:2:G:H22	5:H:101:GOL:C1	2.30	0.45
1:C:14:VAL:CG1	1:C:149:ARG:HB3	2.47	0.45
1:A:115:TYR:N	1:A:128:ASP:OD1	2.51	0.44
1:C:130:THR:N	1:C:131:PRO:HD2	2.32	0.43
2:B:34:C:C3'	2:B:35:A:H5''	2.48	0.42
3:H:1:G:H3'	3:H:2:G:C5'	2.50	0.42
1:F:31:LEU:HD12	1:F:86:VAL:CG1	2.49	0.41
1:C:398:HIS:HD2	2:D:23:C:H5''	1.85	0.41
1:F:203:VAL:HG23	7:F:626:HOH:O	2.20	0.41
1:E:305:PHE:CE2	1:E:315:PRO:HB2	2.56	0.41
2:B:34:C:H2'	2:B:35:A:C4'	2.50	0.41
1:F:14:VAL:CG1	1:F:149:ARG:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:TYR:OH	2:D:33:C:O2	2.35	0.41
1:E:67:PRO:HG2	1:E:70:PHE:CE1	2.56	0.41
1:C:381:LYS:H	6:C:501:PEG:C4	2.34	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	431/457 (94%)	409 (95%)	22 (5%)	0	100	100
1	C	435/457 (95%)	411 (94%)	23 (5%)	1 (0%)	47	73
1	E	436/457 (95%)	424 (97%)	11 (2%)	1 (0%)	47	73
1	F	434/457 (95%)	422 (97%)	11 (2%)	1 (0%)	47	73
All	All	1736/1828 (95%)	1666 (96%)	67 (4%)	3 (0%)	47	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	GLU
1	F	95	ALA
1	E	96	GLU

### 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	386/404 (96%)	383 (99%)	3 (1%)	81	93
1	C	386/404 (96%)	382 (99%)	4 (1%)	76	91
1	E	388/404 (96%)	387 (100%)	1 (0%)	92	98
1	F	386/404 (96%)	385 (100%)	1 (0%)	92	98
All	All	1546/1616 (96%)	1537 (99%)	9 (1%)	86	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	129	ARG
1	A	362	ASN
1	C	42	TYR
1	C	94	TYR
1	C	96	GLU
1	C	411	TYR
1	E	399	THR
1	F	88	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	29/37 (78%)	3 (10%)	0
2	D	23/37 (62%)	1 (4%)	0
2	G	16/37 (43%)	2 (12%)	0
3	H	1/2 (50%)	1 (100%)	0
All	All	69/113 (61%)	7 (10%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	35	A
2	B	36	C
2	B	37	C

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Mol	Chain	Res	Type
2	D	2	G
2	G	5	C
2	G	28	U
3	H	2	G

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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$
4	APC	F	501	-	27,33,33	2.26	9 (33%)	31,52,52	1.66	6 (19%)
5	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.26	0
6	PEG	E	502	-	6,6,6	0.65	0	5,5,5	0.47	0
4	APC	A	501	-	27,33,33	2.24	7 (25%)	31,52,52	1.38	3 (9%)
5	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.41	0
5	GOL	H	101	-	5,5,5	0.35	0	5,5,5	0.33	0
6	PEG	C	501	-	6,6,6	0.62	0	5,5,5	0.33	0
5	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.29	0
5	GOL	E	501	-	5,5,5	0.36	0	5,5,5	0.34	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
4	APC	F	501	-	-	4/15/38/38	0/3/3/3
5	GOL	A	503	-	-	2/4/4/4	-
6	PEG	E	502	-	-	3/4/4/4	-
4	APC	A	501	-	-	2/15/38/38	0/3/3/3
5	GOL	A	504	-	-	4/4/4/4	-
5	GOL	H	101	-	-	0/4/4/4	-
6	PEG	C	501	-	-	1/4/4/4	-
5	GOL	A	502	-	-	2/4/4/4	-
5	GOL	E	501	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	APC	O4'-C1'	7.87	1.52	1.41
4	F	501	APC	O4'-C1'	7.36	1.51	1.41
4	A	501	APC	C2'-C1'	-4.11	1.47	1.53
4	F	501	APC	C2'-C1'	-3.76	1.48	1.53
4	F	501	APC	C2'-C3'	-3.37	1.44	1.53
4	A	501	APC	C2'-C3'	-3.16	1.44	1.53
4	F	501	APC	PA-O2A	-3.16	1.49	1.56
4	F	501	APC	O4'-C4'	3.08	1.51	1.45
4	A	501	APC	C2-N3	3.02	1.37	1.32
4	F	501	APC	C2-N3	2.94	1.36	1.32
4	A	501	APC	O4'-C4'	2.79	1.51	1.45
4	A	501	APC	PB-O2B	-2.43	1.50	1.56
4	F	501	APC	PB-O2B	-2.05	1.51	1.56
4	F	501	APC	PB-O3B	-2.05	1.56	1.58
4	F	501	APC	C5-N7	-2.03	1.32	1.39
4	A	501	APC	C6-N6	2.01	1.41	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	APC	N3-C2-N1	-5.21	120.54	128.68
4	A	501	APC	N3-C2-N1	-5.03	120.82	128.68
4	A	501	APC	C3'-C2'-C1'	3.41	106.12	100.98
4	F	501	APC	C3'-C2'-C1'	2.81	105.21	100.98
4	F	501	APC	PG-O3B-PB	-2.69	123.15	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	APC	C2'-C3'-C4'	2.43	107.37	102.64
4	A	501	APC	C4-C5-N7	-2.30	107.00	109.40
4	F	501	APC	C4-C5-N7	-2.19	107.11	109.40
4	F	501	APC	O3G-PG-O3B	2.03	111.45	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	GOL	O1-C1-C2-C3
4	F	501	APC	C4'-C5'-O5'-PA
4	F	501	APC	C5'-O5'-PA-C3A
5	A	504	GOL	O1-C1-C2-C3
5	A	504	GOL	C1-C2-C3-O3
6	E	502	PEG	O2-C3-C4-O4
5	A	503	GOL	O1-C1-C2-O2
5	A	504	GOL	O2-C2-C3-O3
6	E	502	PEG	O1-C1-C2-O2
5	A	504	GOL	O1-C1-C2-O2
4	F	501	APC	C5'-O5'-PA-O1A
4	A	501	APC	O4'-C4'-C5'-O5'
5	A	502	GOL	O1-C1-C2-O2
6	C	501	PEG	O1-C1-C2-O2
4	F	501	APC	PB-C3A-PA-O1A
4	A	501	APC	C3'-C4'-C5'-O5'
5	A	502	GOL	C1-C2-C3-O3
6	E	502	PEG	C1-C2-O2-C3

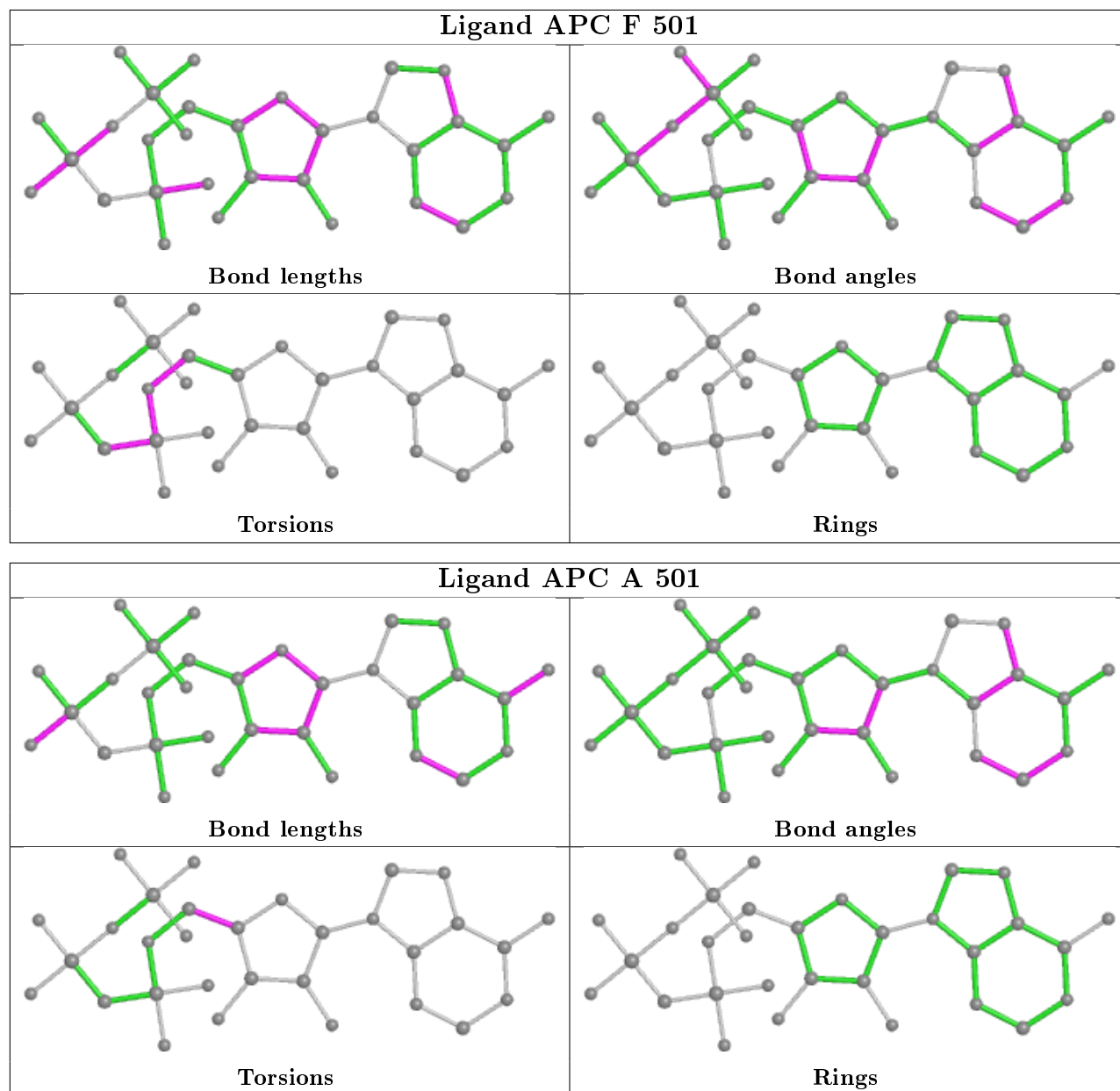
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	501	APC	4	0
4	A	501	APC	1	0
5	H	101	GOL	1	0
6	C	501	PEG	2	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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	435/457 (95%)	0.42	35 (8%) 12 10	34, 70, 159, 219	0
1	C	437/457 (95%)	0.78	61 (13%) 2 1	36, 78, 180, 280	0
1	E	437/457 (95%)	0.19	16 (3%) 41 41	35, 58, 104, 160	0
1	F	436/457 (95%)	0.18	14 (3%) 47 48	40, 60, 102, 160	0
2	B	31/37 (83%)	2.45	16 (51%) 0 0	113, 146, 280, 423	0
2	D	26/37 (70%)	2.99	20 (76%) 0 0	143, 171, 199, 254	0
2	G	18/37 (48%)	0.74	3 (16%) 1 1	75, 88, 157, 159	0
3	H	2/2 (100%)	3.15	2 (100%) 0 0	148, 148, 148, 161	0
All	All	1822/1941 (93%)	0.47	167 (9%) 9 7	34, 66, 162, 423	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	10.3
1	C	92	ILE	10.0
1	C	115	TYR	8.7
1	C	73	GLU	8.0
1	C	68	GLU	7.8
1	C	1	MET	7.4
1	C	77	GLU	7.3
2	B	37	C	7.1
1	A	1	MET	6.8
1	A	78	ARG	6.6
2	B	7	G	6.6
2	B	35	A	5.7
2	B	8	C	5.7
2	B	36	C	5.2
2	D	7	G	5.1
1	E	124	LYS	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	122	ASN	5.0
1	E	123	ILE	5.0
2	D	9	G	4.9
1	C	93	ARG	4.7
1	C	84	LYS	4.7
2	B	18	G	4.6
2	D	20	C	4.6
1	C	81	GLU	4.6
2	D	25	C	4.5
2	G	9	G	4.4
2	D	10	G	4.3
1	F	124	LYS	4.3
1	F	260	LEU	4.2
1	A	61	ASP	4.2
1	A	72	LYS	4.2
2	D	6	U	4.1
1	C	76	ARG	4.1
2	B	19	U	4.0
1	C	22	ARG	4.0
1	A	74	GLU	4.0
1	A	82	ILE	4.0
1	F	123	ILE	3.9
2	B	6	U	3.9
1	A	81	GLU	3.8
2	B	31	U	3.8
2	D	16	G	3.7
1	A	98	PRO	3.7
1	E	258	HIS	3.7
2	D	24	G	3.7
1	E	259	PRO	3.7
1	C	105	LYS	3.7
1	A	33	ARG	3.7
2	D	4	G	3.6
1	C	123	ILE	3.6
1	F	261	GLU	3.6
1	E	175	CYS	3.5
1	C	72	LYS	3.5
1	C	78	ARG	3.5
1	E	3	VAL	3.5
1	C	120	PRO	3.4
3	H	1	G	3.4
1	C	94	TYR	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	2	G	3.4
1	A	75	LEU	3.4
2	D	21	C	3.4
1	C	75	LEU	3.3
1	C	117	LEU	3.3
1	C	114	CYS	3.3
1	C	260	LEU	3.2
2	G	1	G	3.2
2	D	31	U	3.1
1	C	39	GLY	3.1
1	C	61	ASP	3.1
2	B	9	G	3.0
1	C	85	ALA	3.0
1	A	73	GLU	3.0
2	D	1	G	3.0
1	C	26	GLU	2.9
1	A	70	PHE	2.9
1	C	98	PRO	2.9
3	H	2	G	2.9
1	C	259	PRO	2.9
1	A	122	ASN	2.9
1	C	119	GLU	2.8
1	E	97	HIS	2.8
1	C	12	GLU	2.8
1	F	96	GLU	2.8
1	F	119	GLU	2.8
1	A	100	VAL	2.8
1	C	116	LYS	2.8
1	E	361	ARG	2.8
1	C	2	LYS	2.7
2	D	32	G	2.7
2	D	33	C	2.7
1	C	69	GLU	2.7
1	F	122	ASN	2.7
1	C	66	PHE	2.7
1	A	69	GLU	2.7
2	D	15	C	2.7
1	A	117	LEU	2.7
1	C	58	LEU	2.7
1	C	59	GLU	2.6
1	C	15	ILE	2.6
1	C	109	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	289	VAL	2.6
1	F	356	LYS	2.6
1	C	91	GLU	2.6
1	A	90	TYR	2.6
1	E	122	ASN	2.5
1	C	263	GLU	2.5
1	A	46	GLY	2.5
2	D	8	C	2.5
1	A	17	ASP	2.5
1	F	25	ARG	2.5
2	D	3	C	2.5
1	E	353	ARG	2.5
1	A	172	GLY	2.5
1	C	287	ASP	2.5
1	C	130	THR	2.4
1	A	22	ARG	2.4
1	A	60	ILE	2.4
1	C	89	SER	2.4
1	C	102	GLY	2.3
1	C	18	GLU	2.3
1	C	82	ILE	2.3
2	B	11	G	2.3
1	A	119	GLU	2.3
1	C	40	VAL	2.3
1	A	259	PRO	2.3
1	C	64	LEU	2.3
2	D	22	C	2.3
1	C	103	VAL	2.3
2	B	5	C	2.3
2	D	5	C	2.3
1	A	324	GLU	2.3
1	A	71	SER	2.3
1	C	113	PRO	2.3
2	B	1	G	2.3
1	A	92	ILE	2.3
1	C	9	LYS	2.3
1	C	35	LEU	2.2
2	B	10	G	2.2
1	A	48	TYR	2.2
1	A	37	GLU	2.2
2	G	23	C	2.2
2	B	17	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	96	GLU	2.2
1	A	115	TYR	2.2
2	B	34	C	2.2
1	C	46	GLY	2.2
1	C	43	VAL	2.2
1	E	260	LEU	2.2
1	E	118	LYS	2.1
1	A	36	ASP	2.1
1	F	95	ALA	2.1
1	F	97	HIS	2.1
1	C	25	ARG	2.1
1	F	76	ARG	2.1
1	C	217	VAL	2.1
1	C	7	LEU	2.1
1	E	318	SER	2.1
1	A	223	LYS	2.1
1	A	111	VAL	2.1
1	C	124	LYS	2.1
1	E	1	MET	2.1
1	F	179	ILE	2.0
1	F	46	GLY	2.0
1	C	251	LEU	2.0
1	A	19	GLU	2.0
1	C	37	GLU	2.0
1	E	171	SER	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](#)

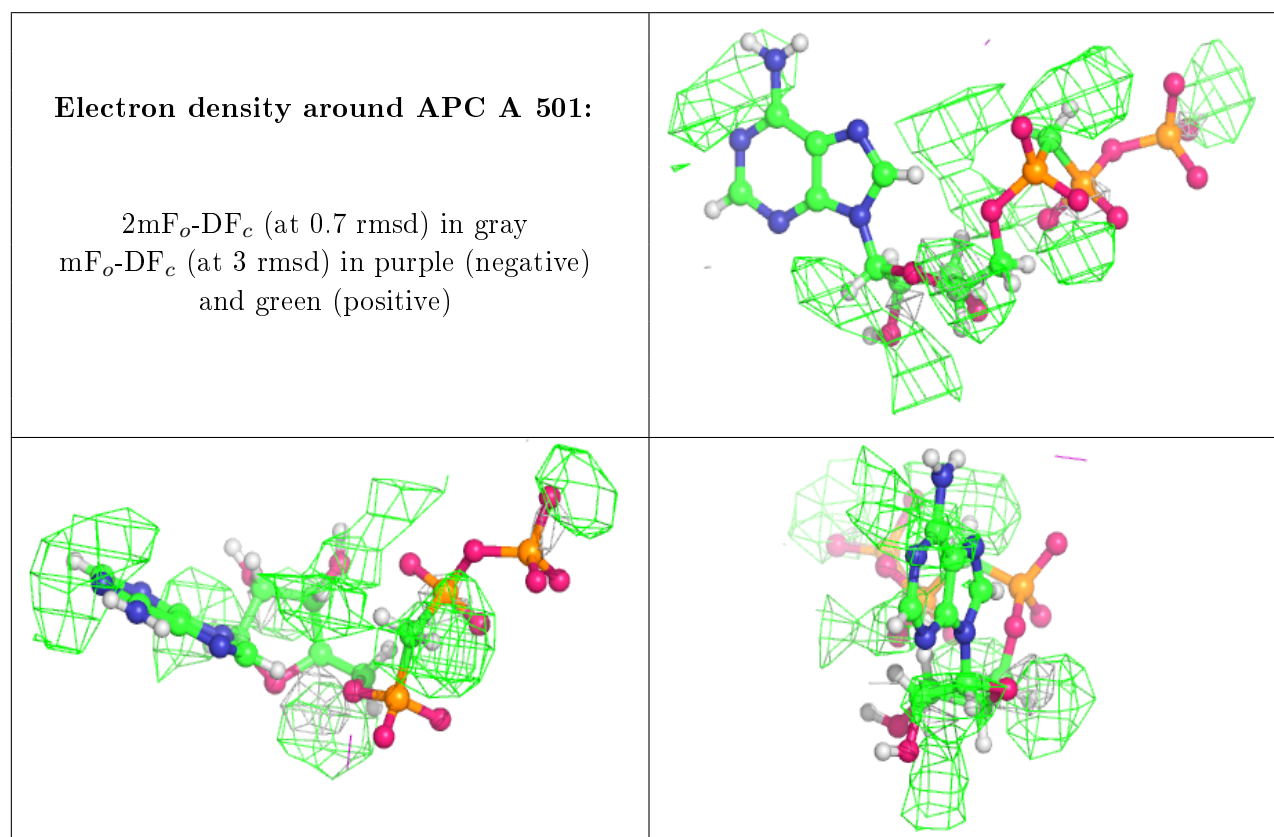
There are no carbohydrates in this entry.

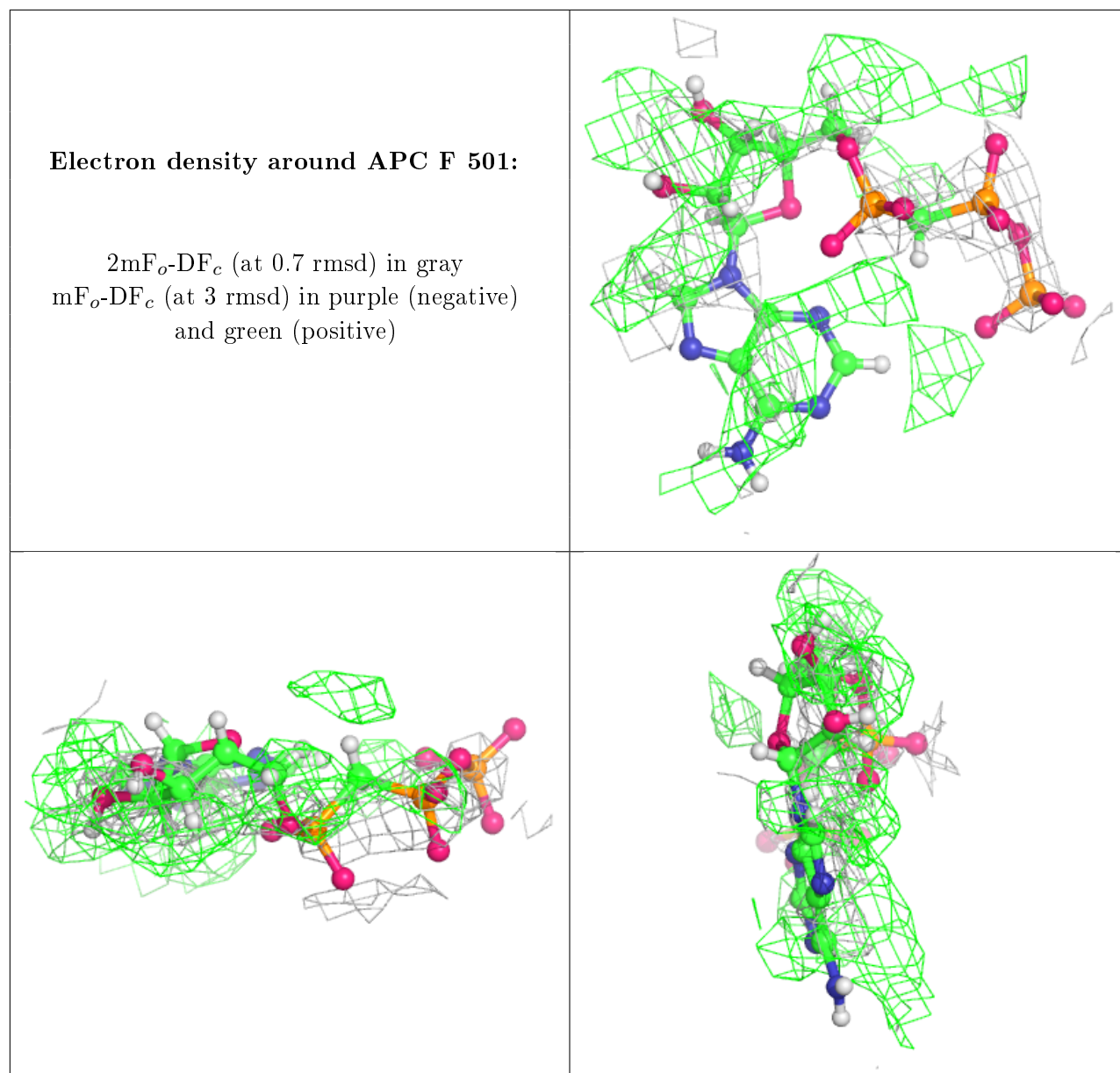
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	APC	A	501	31/31	0.49	0.70	51,73,86,92	45
4	APC	F	501	31/31	0.62	0.63	46,70,84,91	45
5	GOL	H	101	6/6	0.67	0.49	64,77,82,85	14
5	GOL	A	503	6/6	0.71	0.51	84,101,113,116	0
5	GOL	A	504	6/6	0.77	0.57	87,106,117,128	0
6	PEG	C	501	7/7	0.83	0.36	89,107,124,127	0
5	GOL	A	502	6/6	0.85	0.26	82,98,111,114	0
5	GOL	E	501	6/6	0.87	0.23	80,97,114,116	0
6	PEG	E	502	7/7	0.90	0.28	74,90,93,95	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.