



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2020 – 12:45 pm GMT

PDB ID : 6YAK  
Title : Split gene transketolase, active alpha2beta2 heterotetramer  
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Deposited on : 2020-03-12  
Resolution : 1.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.14.6  
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) : 2.14.6

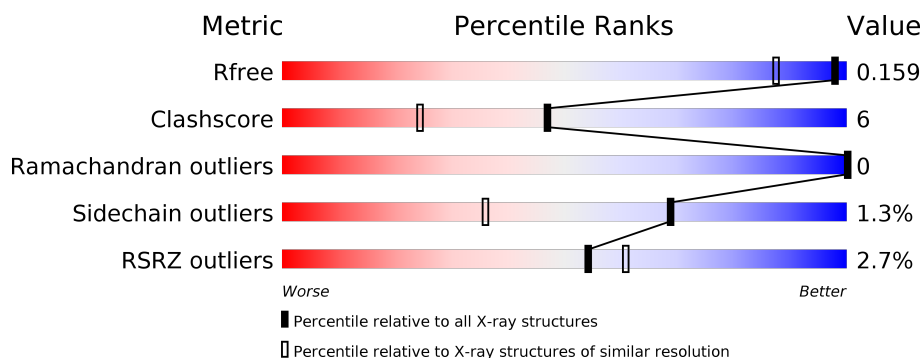
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	AAA	309	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	CCC	309	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
2	BBB	341	<div> <div></div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
2	DDD	341	<div> <div></div> <div> <div></div> <div>84%</div> <div>8%</div> <div>9%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	LMR	AAA	306	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21938 atoms, of which 10460 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.

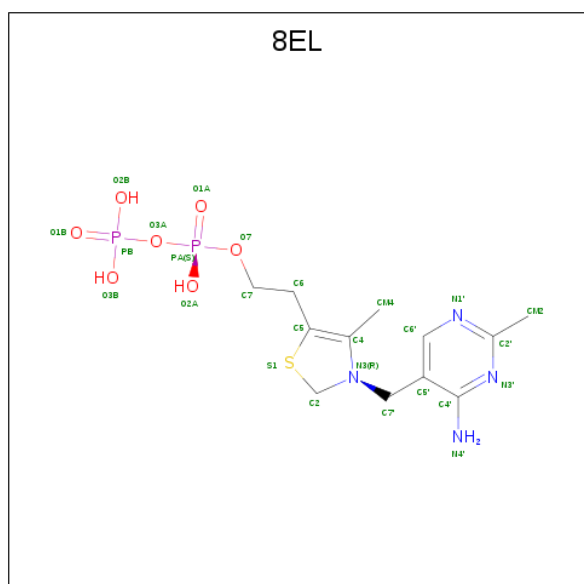
- Molecule 1 is a protein called N-terminal component of the split chain transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	282	Total	C	H	N	O	S	105	32	0
			4834	1523	2459	414	427	11			
1	CCC	282	Total	C	H	N	O	S	104	37	0
			4894	1548	2495	412	428	11			

- Molecule 2 is a protein called C-terminal component of the split chain transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	311	Total	C	H	N	O	S	83	40	0
			5216	1627	2689	421	471	8			
2	DDD	311	Total	C	H	N	O	S	81	43	0
			5270	1642	2721	425	474	8			

- Molecule 3 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2H-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: 8EL) (formula: C<sub>12</sub>H<sub>20</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by author).

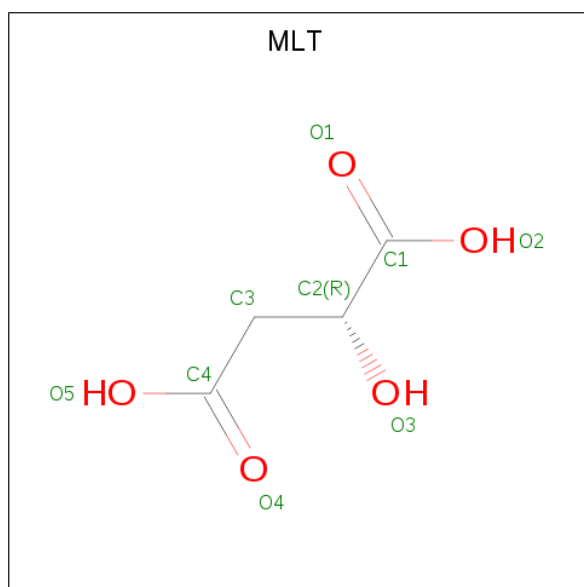


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
3	CCC	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	2	Total Ca 2 2	0	0
4	AAA	2	Total Ca 2 2	0	0

- Molecule 5 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



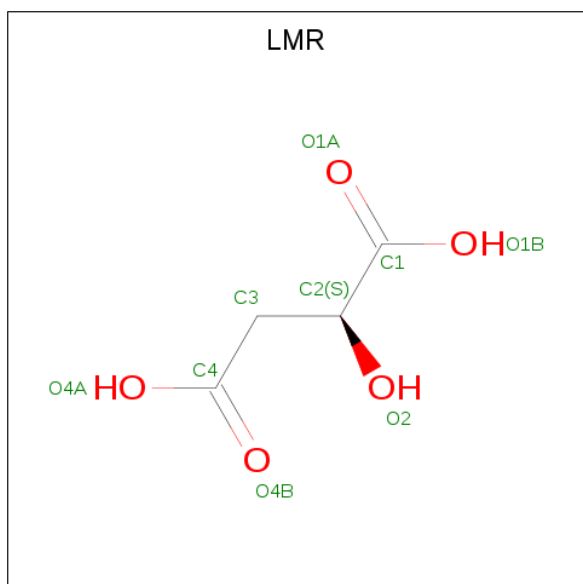
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			13	4	4	5		
5	AAA	1	Total	C	H	O	1	0
			13	4	4	5		
5	BBB	1	Total	C	H	O	1	0
			13	4	4	5		
5	BBB	1	Total	C	H	O	1	0
			13	4	4	5		
5	BBB	1	Total	C	H	O	1	0
			13	4	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	BBB	1	Total	C	H	O	1	0
			13	4	4	5		
5	CCC	1	Total	C	H	O	1	0
			13	4	4	5		
5	CCC	1	Total	C	H	O	1	0
			13	4	4	5		
5	CCC	1	Total	C	H	O	1	0
			13	4	4	5		
5	CCC	1	Total	C	H	O	1	0
			13	4	4	5		

- Molecule 6 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			13	4	4	5		
6	AAA	1	Total	C	H	O	1	0
			13	4	4	5		
6	AAA	1	Total	C	H	O	1	0
			13	4	4	5		
6	DDD	1	Total	C	H	O	1	0
			13	4	4	5		
6	DDD	1	Total	C	H	O	1	0
			13	4	4	5		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total 1	Cl 1	0	0
7	BBB	1	Total 1	Cl 1	0	0
7	DDD	1	Total 1	Cl 1	0	0
7	AAA	1	Total 1	Cl 1	0	0

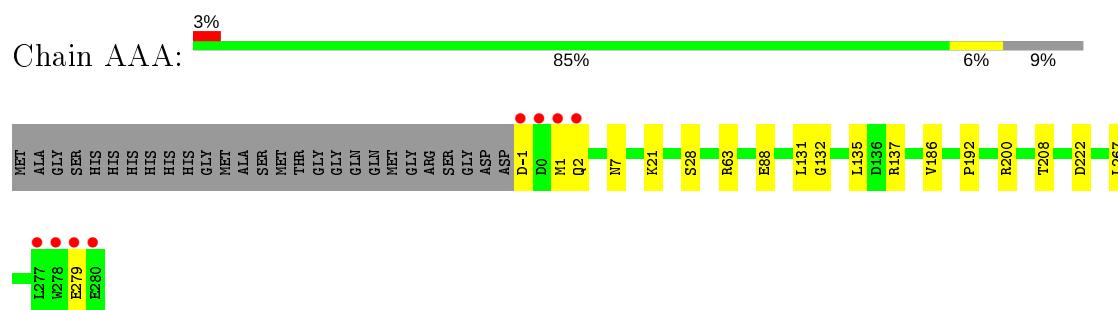
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	376	Total 376	O 376	0	0
8	BBB	366	Total 366	O 366	0	0
8	CCC	343	Total 343	O 343	0	0
8	DDD	339	Total 339	O 339	0	0

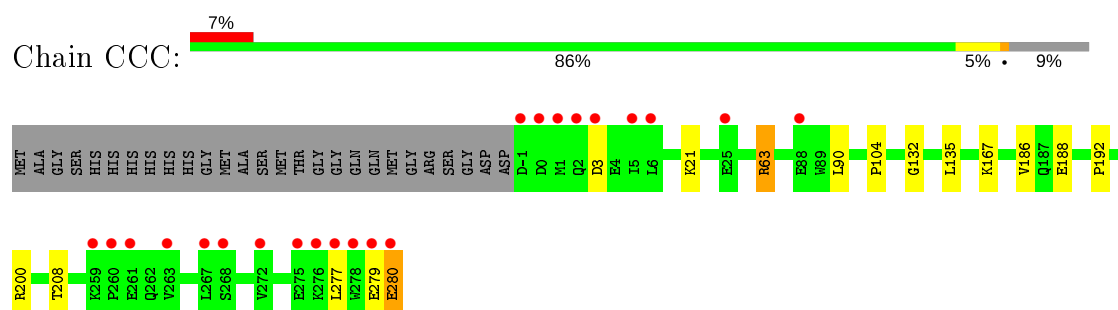
### 3 Residue-property plots [i](#)

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.

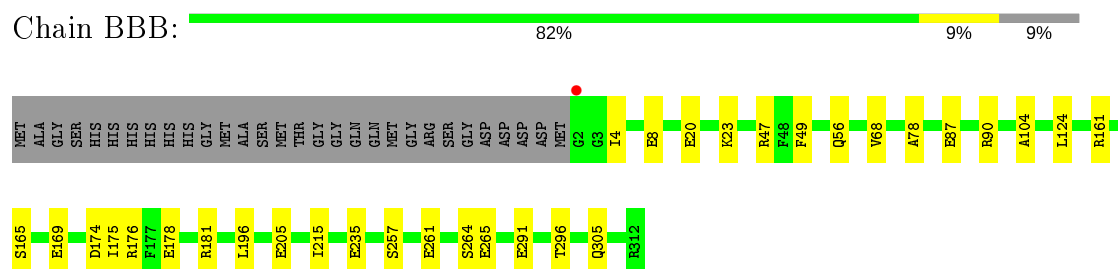
- Molecule 1: N-terminal component of the split chain transketolase



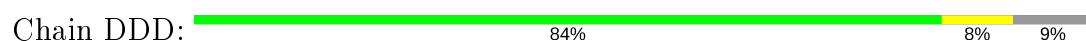
- Molecule 1: N-terminal component of the split chain transketolase



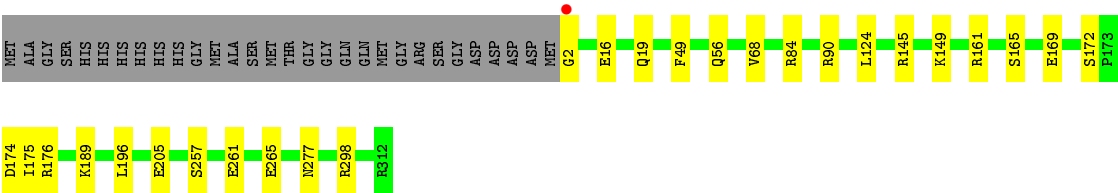
- Molecule 2: C-terminal component of the split chain transketolase



- Molecule 2: C-terminal component of the split chain transketolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.08Å 130.05Å 165.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.87 – 1.34 60.80 – 1.34	Depositor EDS
% Data completeness (in resolution range)	97.6 (60.87-1.34) 97.6 (60.80-1.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.34Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.141 , 0.159 0.141 , 0.159	Depositor DCC
$R_{free}$ test set	14402 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	21938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 8EL, LMR, CA, MLT, CL

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	AAA	0.66	0/2508	0.76	0/3385
1	CCC	0.64	0/2561	0.73	0/3456
2	BBB	0.64	0/2679	0.75	3/3615 (0.1%)
2	DDD	0.65	0/2709	0.73	0/3652
All	All	0.65	0/10457	0.74	3/14108 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	47	ARG	NE-CZ-NH1	6.85	123.73	120.30
2	BBB	47	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	BBB	90	ARG	NE-CZ-NH1	-5.06	117.77	120.30

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	AAA	2375	2459	2481	28	0
1	CCC	2399	2495	2526	17	0
2	BBB	2527	2689	2721	55	0
2	DDD	2549	2721	2757	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	26	16	0	0	0
3	CCC	26	16	0	0	0
4	AAA	2	0	0	0	0
4	CCC	2	0	0	0	0
5	AAA	18	8	8	1	0
5	BBB	36	16	16	3	0
5	CCC	45	20	20	2	0
6	AAA	27	12	12	11	0
6	DDD	18	8	8	0	0
7	AAA	1	0	0	0	0
7	BBB	1	0	0	0	0
7	CCC	1	0	0	0	0
7	DDD	1	0	0	0	0
8	AAA	376	0	0	13	1
8	BBB	366	0	0	23	2
8	CCC	343	0	0	6	0
8	DDD	339	0	0	12	0
All	All	11478	10460	10549	128	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (128) 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)
2:BBB:176[B]:ARG:NH2	2:BBB:181[B]:ARG:HH12	1.16	1.39
2:BBB:56[A]:GLN:NE2	2:DDD:56[A]:GLN:NE2	1.82	1.24
2:BBB:165[B]:SER:OG	8:BBB:603:HOH:O	1.57	1.20
2:BBB:174[B]:ASP:OD2	8:BBB:605:HOH:O	1.62	1.18
1:AAA:137[B]:ARG:NH1	6:AAA:306:LMR:O1B	1.79	1.16
2:BBB:265[B]:GLU:OE1	8:BBB:604:HOH:O	1.61	1.16
2:BBB:165[A]:SER:HB3	8:BBB:603:HOH:O	1.43	1.14
2:BBB:176[B]:ARG:NH2	2:BBB:181[B]:ARG:NH1	1.96	1.12
1:AAA:208[B]:THR:HG23	8:AAA:607:HOH:O	1.55	1.06
1:AAA:137[A]:ARG:HG2	6:AAA:306:LMR:C4	1.85	1.06
2:BBB:176[B]:ARG:HH21	2:BBB:178[B]:GLU:HG3	1.18	1.05
2:BBB:56[A]:GLN:HE22	2:DDD:56[A]:GLN:NE2	1.55	1.03
2:DDD:176[B]:ARG:HH21	2:DDD:176[B]:ARG:HG2	1.20	1.02
2:DDD:176[B]:ARG:CG	2:DDD:176[B]:ARG:HH21	1.74	0.99
2:DDD:165[A]:SER:OG	8:DDD:1504:HOH:O	1.80	0.99
2:BBB:56[A]:GLN:NE2	2:DDD:56[A]:GLN:HE22	1.57	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:222[B]:ASP:OD1	8:AAA:403:HOH:O	1.81	0.98
2:BBB:165[A]:SER:OG	8:BBB:606:HOH:O	1.83	0.96
2:DDD:172[B]:SER:OG	2:DDD:174[B]:ASP:OD1	1.88	0.89
1:AAA:208[B]:THR:CG2	8:AAA:607:HOH:O	2.15	0.89
2:BBB:176[B]:ARG:NH2	2:BBB:178[B]:GLU:HG3	1.86	0.89
2:DDD:298[B]:ARG:HD2	8:DDD:1704:HOH:O	1.72	0.88
1:AAA:137[A]:ARG:HG2	6:AAA:306:LMR:O4B	1.73	0.87
2:BBB:291[B]:GLU:HG3	8:BBB:664:HOH:O	1.74	0.87
2:BBB:176[B]:ARG:HH22	2:BBB:181[B]:ARG:NH1	1.63	0.85
2:BBB:176[B]:ARG:CZ	2:BBB:181[B]:ARG:HH22	1.91	0.83
2:DDD:298[B]:ARG:HG2	2:DDD:298[B]:ARG:HH21	1.41	0.82
2:BBB:176[B]:ARG:HH22	2:BBB:181[B]:ARG:HH12	0.86	0.82
2:BBB:176[B]:ARG:HH21	2:BBB:181[B]:ARG:HH12	1.31	0.79
2:BBB:176[B]:ARG:HH21	2:BBB:178[B]:GLU:CG	1.96	0.79
2:BBB:20[B]:GLU:CG	8:BBB:826:HOH:O	2.31	0.78
6:AAA:307:LMR:O1B	8:AAA:404:HOH:O	2.02	0.77
2:DDD:19:GLN:O	8:DDD:1506:HOH:O	2.03	0.77
2:DDD:277[B]:ASN:OD1	8:DDD:1507:HOH:O	2.04	0.76
1:CCC:63[B]:ARG:NH1	2:DDD:68[B]:VAL:HG12	2.02	0.75
2:BBB:235[A]:GLU:HG3	8:BBB:879:HOH:O	1.85	0.75
2:BBB:257[B]:SER:OG	2:DDD:261:GLU:OE2	2.05	0.74
1:AAA:186[B]:VAL:HG12	1:AAA:192:PRO:HD3	1.68	0.74
2:DDD:298[B]:ARG:HG2	2:DDD:298[B]:ARG:NH2	2.03	0.73
2:BBB:20[B]:GLU:HG3	8:BBB:826:HOH:O	1.89	0.72
2:BBB:305[B]:GLN:OE1	8:BBB:607:HOH:O	2.09	0.70
2:DDD:298[B]:ARG:NH1	8:DDD:1509:HOH:O	2.24	0.69
1:AAA:137[B]:ARG:HE	6:AAA:306:LMR:H3A	1.57	0.68
1:AAA:28:SER:HB2	8:AAA:565:HOH:O	1.93	0.68
2:DDD:176[B]:ARG:CG	2:DDD:176[B]:ARG:NH2	2.43	0.68
2:BBB:178[B]:GLU:HG3	2:BBB:181[B]:ARG:NH1	2.10	0.66
2:DDD:176[B]:ARG:NH2	2:DDD:176[B]:ARG:HG2	2.02	0.65
2:BBB:264[B]:SER:OG	8:DDD:1501:HOH:O	2.15	0.65
1:CCC:167[B]:LYS:HD3	8:CCC:550:HOH:O	1.97	0.64
1:CCC:208[B]:THR:HG23	8:CCC:566:HOH:O	1.96	0.64
2:BBB:165[B]:SER:CB	8:BBB:603:HOH:O	2.32	0.64
2:BBB:176[B]:ARG:NH2	2:BBB:181[B]:ARG:CZ	2.61	0.63
1:CCC:186[B]:VAL:HG12	1:CCC:192:PRO:CD	2.29	0.63
2:BBB:205[A]:GLU:HG2	8:BBB:805:HOH:O	2.00	0.61
1:CCC:186[B]:VAL:HG12	1:CCC:192:PRO:HD3	1.83	0.59
2:DDD:205[A]:GLU:HG3	8:DDD:1518:HOH:O	2.02	0.59
1:AAA:63[B]:ARG:NH1	8:AAA:405:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:186[B]:VAL:HG12	1:AAA:192:PRO:CD	2.32	0.58
1:CCC:188[B]:GLU:OE2	8:CCC:402:HOH:O	2.17	0.58
1:CCC:167[B]:LYS:HE2	8:CCC:432:HOH:O	2.03	0.58
2:BBB:176[B]:ARG:NH2	2:BBB:181[B]:ARG:HH22	2.01	0.57
2:BBB:176[B]:ARG:HD2	8:BBB:810:HOH:O	2.04	0.57
2:BBB:56[A]:GLN:HE21	2:DDD:56[A]:GLN:NE2	1.96	0.57
1:AAA:88[B]:GLU:HG3	8:AAA:552:HOH:O	2.04	0.56
1:CCC:104:PRO:HB2	8:CCC:418:HOH:O	2.04	0.56
2:BBB:205[A]:GLU:CD	8:BBB:622:HOH:O	2.43	0.56
5:BBB:504:MLT:H31	8:BBB:664:HOH:O	2.07	0.55
2:BBB:176[B]:ARG:NH2	2:BBB:181[B]:ARG:NH2	2.56	0.54
1:AAA:137[A]:ARG:HA	6:AAA:306:LMR:O4B	2.07	0.54
1:AAA:137[B]:ARG:HA	6:AAA:306:LMR:O4B	2.07	0.54
2:BBB:178[B]:GLU:HG3	2:BBB:181[B]:ARG:CZ	2.38	0.54
2:BBB:56[A]:GLN:NE2	2:DDD:56[A]:GLN:HE21	1.96	0.54
1:AAA:200[B]:ARG:NH2	8:AAA:407:HOH:O	2.28	0.54
2:BBB:4:ILE:HD12	2:BBB:8[B]:GLU:HG2	1.89	0.54
2:BBB:291[B]:GLU:HG2	8:BBB:875:HOH:O	2.08	0.53
6:AAA:306:LMR:H3A	8:AAA:413:HOH:O	2.10	0.51
1:CCC:200[B]:ARG:NH2	8:CCC:407:HOH:O	2.39	0.51
1:CCC:186[B]:VAL:CG1	1:CCC:192:PRO:HD3	2.41	0.51
1:AAA:137[A]:ARG:CG	6:AAA:306:LMR:O4B	2.53	0.51
6:AAA:306:LMR:O2	6:AAA:306:LMR:O4B	2.13	0.51
2:DDD:176[B]:ARG:NH2	2:DDD:176[B]:ARG:HG3	2.26	0.50
2:BBB:215[B]:ILE:HD11	8:BBB:933:HOH:O	2.12	0.49
2:BBB:176[B]:ARG:HE	2:BBB:178[B]:GLU:CD	2.16	0.48
2:BBB:23[B]:LYS:HD3	8:BBB:665:HOH:O	2.12	0.48
1:AAA:21[A]:LYS:CE	8:AAA:446:HOH:O	2.61	0.47
1:AAA:7[A]:ASN:ND2	8:AAA:420:HOH:O	2.48	0.47
1:CCC:90:LEU:HB2	5:CCC:304:MLT:H2	1.97	0.47
1:AAA:-1:ASP:HB3	1:AAA:2:GLN:HB3	1.97	0.47
1:AAA:137[B]:ARG:HG2	6:AAA:306:LMR:C4	2.44	0.47
1:CCC:135[B]:LEU:HD11	2:DDD:49:PHE:CZ	2.50	0.47
2:DDD:265[B]:GLU:HG2	8:DDD:1559:HOH:O	2.14	0.47
1:AAA:137[B]:ARG:NH1	8:AAA:413:HOH:O	2.33	0.46
2:BBB:296:THR:OG1	5:BBB:504:MLT:H32	2.15	0.46
2:BBB:291[B]:GLU:CG	8:BBB:664:HOH:O	2.48	0.46
2:BBB:56[A]:GLN:HE22	2:DDD:56[A]:GLN:HE21	1.54	0.45
2:BBB:20[B]:GLU:HG2	8:BBB:826:HOH:O	2.09	0.45
1:AAA:186[B]:VAL:CG1	1:AAA:192:PRO:HD3	2.42	0.45
1:AAA:132:GLY:O	1:AAA:135[B]:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:63[B]:ARG:CZ	2:DDD:68[B]:VAL:HG12	2.47	0.45
5:AAA:304:MLT:O5	5:AAA:304:MLT:O3	2.33	0.44
1:CCC:277:LEU:O	1:CCC:280:GLU:HG3	2.18	0.43
2:DDD:298[B]:ARG:HH21	2:DDD:298[B]:ARG:CG	2.18	0.43
2:BBB:176[B]:ARG:NE	2:BBB:178[B]:GLU:OE2	2.41	0.43
2:DDD:16[A]:GLU:CD	2:DDD:149:LYS:HE3	2.39	0.43
2:BBB:261:GLU:OE2	2:DDD:257[B]:SER:OG	2.18	0.43
1:AAA:131:LEU:O	1:AAA:135[B]:LEU:HG	2.19	0.42
1:CCC:21[A]:LYS:HG2	5:CCC:304:MLT:O5	2.19	0.42
2:BBB:169[B]:GLU:HG2	8:BBB:811:HOH:O	2.19	0.42
2:BBB:176[B]:ARG:NH2	2:BBB:178[B]:GLU:CG	2.68	0.42
2:DDD:145:ARG:NH1	8:DDD:1516:HOH:O	2.51	0.42
1:AAA:21[A]:LYS:HE3	1:AAA:267:LEU:HD13	2.02	0.41
2:DDD:165[B]:SER:HB2	8:DDD:1504:HOH:O	2.20	0.41
2:BBB:8[B]:GLU:HG3	8:BBB:886:HOH:O	2.19	0.41
1:CCC:186[B]:VAL:CG1	1:CCC:192:PRO:CD	2.97	0.41
2:DDD:124:LEU:HD21	2:DDD:161:ARG:HD2	2.03	0.41
1:AAA:135[B]:LEU:HD11	2:BBB:49:PHE:CZ	2.56	0.41
2:DDD:2:GLY:N	8:DDD:1519:HOH:O	2.53	0.41
2:BBB:78:ALA:HA	2:BBB:104:ALA:HB1	2.02	0.41
1:CCC:132:GLY:HA3	2:DDD:68[B]:VAL:HG21	2.03	0.41
2:BBB:87:GLU:OE2	2:DDD:84[A]:ARG:HD3	2.21	0.41
1:AAA:63[B]:ARG:HH21	1:AAA:63[B]:ARG:HD2	1.76	0.40
2:BBB:181[A]:ARG:NH2	8:BBB:634:HOH:O	2.53	0.40
5:BBB:502:MLT:O3	5:BBB:502:MLT:O4	2.37	0.40
2:BBB:124:LEU:HD21	2:BBB:161:ARG:HD2	2.03	0.40
1:AAA:222[B]:ASP:CG	8:AAA:403:HOH:O	2.46	0.40
2:DDD:169[B]:GLU:HG2	8:DDD:1772:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BBB:945:HOH:O	8:BBB:945:HOH:O[4_556]	1.97	0.23
8:AAA:478:HOH:O	8:BBB:948:HOH:O[2_555]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	312/309 (101%)	305 (98%)	7 (2%)	0	100	100
1	CCC	317/309 (103%)	311 (98%)	6 (2%)	0	100	100
2	BBB	349/341 (102%)	339 (97%)	10 (3%)	0	100	100
2	DDD	352/341 (103%)	340 (97%)	12 (3%)	0	100	100
All	All	1330/1300 (102%)	1295 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	262/249 (105%)	260 (99%)	2 (1%)	81	57
1	CCC	267/249 (107%)	261 (98%)	6 (2%)	52	17
2	BBB	277/260 (106%)	275 (99%)	2 (1%)	84	62
2	DDD	280/260 (108%)	275 (98%)	5 (2%)	59	24
All	All	1086/1018 (107%)	1071 (99%)	15 (1%)	69	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	MET
1	AAA	279	GLU

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Mol	Chain	Res	Type
2	BBB	175	ILE
2	BBB	196	LEU
1	CCC	3[A]	ASP
1	CCC	3[B]	ASP
1	CCC	63[A]	ARG
1	CCC	63[B]	ARG
1	CCC	279	GLU
1	CCC	280	GLU
2	DDD	90	ARG
2	DDD	175	ILE
2	DDD	189[A]	LYS
2	DDD	189[B]	LYS
2	DDD	196	LEU

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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
5	MLT	BBB	502	-	2,8,8	0.54	0	3,10,10	1.31	0
6	LMR	AAA	306	-	2,8,8	0.98	0	3,10,10	4.44	2 (66%)
5	MLT	BBB	503	-	2,8,8	0.23	0	3,10,10	1.10	0
5	MLT	CCC	304	-	2,8,8	0.36	0	3,10,10	1.04	0
5	MLT	CCC	307	-	2,8,8	0.33	0	3,10,10	2.69	2 (66%)
6	LMR	AAA	308	-	2,8,8	0.56	0	3,10,10	0.78	0
3	8EL	AAA	301	4	24,27,27	1.07	2 (8%)	30,40,40	0.74	0
6	LMR	DDD	1401	-	2,8,8	0.61	0	3,10,10	0.67	0
6	LMR	AAA	307	-	2,8,8	0.50	0	3,10,10	0.51	0
5	MLT	CCC	306	-	2,8,8	0.37	0	3,10,10	0.40	0
3	8EL	CCC	301	4	24,27,27	1.00	1 (4%)	30,40,40	0.82	0
5	MLT	BBB	504	-	2,8,8	0.50	0	3,10,10	1.62	1 (33%)
5	MLT	AAA	305	-	2,8,8	0.17	0	3,10,10	1.31	1 (33%)
5	MLT	CCC	308	-	2,8,8	0.30	0	3,10,10	0.91	0
5	MLT	CCC	305	-	2,8,8	0.29	0	3,10,10	0.47	0
5	MLT	AAA	304	-	2,8,8	0.49	0	3,10,10	1.72	1 (33%)
5	MLT	BBB	501	-	2,8,8	0.38	0	3,10,10	0.50	0
6	LMR	DDD	1402	-	2,8,8	0.68	0	3,10,10	1.27	1 (33%)

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
5	MLT	BBB	502	-	-	2/2/8/8	-
6	LMR	AAA	306	-	-	1/2/8/8	-
5	MLT	BBB	503	-	-	0/2/8/8	-
5	MLT	CCC	304	-	-	1/2/8/8	-
5	MLT	CCC	307	-	-	2/2/8/8	-
6	LMR	AAA	308	-	-	0/2/8/8	-
3	8EL	AAA	301	4	-	2/17/30/30	0/2/2/2
6	LMR	DDD	1401	-	-	2/2/8/8	-
6	LMR	AAA	307	-	-	2/2/8/8	-
5	MLT	CCC	306	-	-	0/2/8/8	-
3	8EL	CCC	301	4	-	5/17/30/30	0/2/2/2
5	MLT	BBB	504	-	-	2/2/8/8	-
5	MLT	AAA	305	-	-	2/2/8/8	-
5	MLT	CCC	308	-	-	2/2/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLT	CCC	305	-	-	2/2/8/8	-
5	MLT	AAA	304	-	-	2/2/8/8	-
5	MLT	BBB	501	-	-	0/2/8/8	-
6	LMR	DDD	1402	-	-	2/2/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	301	8EL	C2-N3	-3.67	1.34	1.45
3	CCC	301	8EL	C2-N3	-3.61	1.34	1.45
3	AAA	301	8EL	PB-O3B	-2.32	1.45	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AAA	306	LMR	C3-C2-C1	7.30	120.38	111.10
5	CCC	307	MLT	C3-C2-C1	3.56	115.63	111.10
5	CCC	307	MLT	O3-C2-C1	-2.95	102.79	111.66
6	AAA	306	LMR	O2-C2-C1	-2.35	104.58	111.66
5	AAA	304	MLT	O3-C2-C3	2.28	113.50	108.50
5	BBB	504	MLT	O3-C2-C1	-2.12	105.27	111.66
5	AAA	305	MLT	C3-C2-C1	2.09	113.75	111.10
6	DDD	1402	LMR	C3-C2-C1	2.05	113.70	111.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	306	LMR	O2-C2-C3-C4
5	CCC	307	MLT	C1-C2-C3-C4
5	CCC	307	MLT	O3-C2-C3-C4
3	AAA	301	8EL	PA-O3A-PB-O3B
5	AAA	305	MLT	C1-C2-C3-C4
5	AAA	305	MLT	O3-C2-C3-C4
3	CCC	301	8EL	PA-O3A-PB-O2B
5	BBB	504	MLT	C1-C2-C3-C4
5	BBB	504	MLT	O3-C2-C3-C4
6	DDD	1402	LMR	C1-C2-C3-C4
6	DDD	1402	LMR	O2-C2-C3-C4
5	BBB	502	MLT	C1-C2-C3-C4

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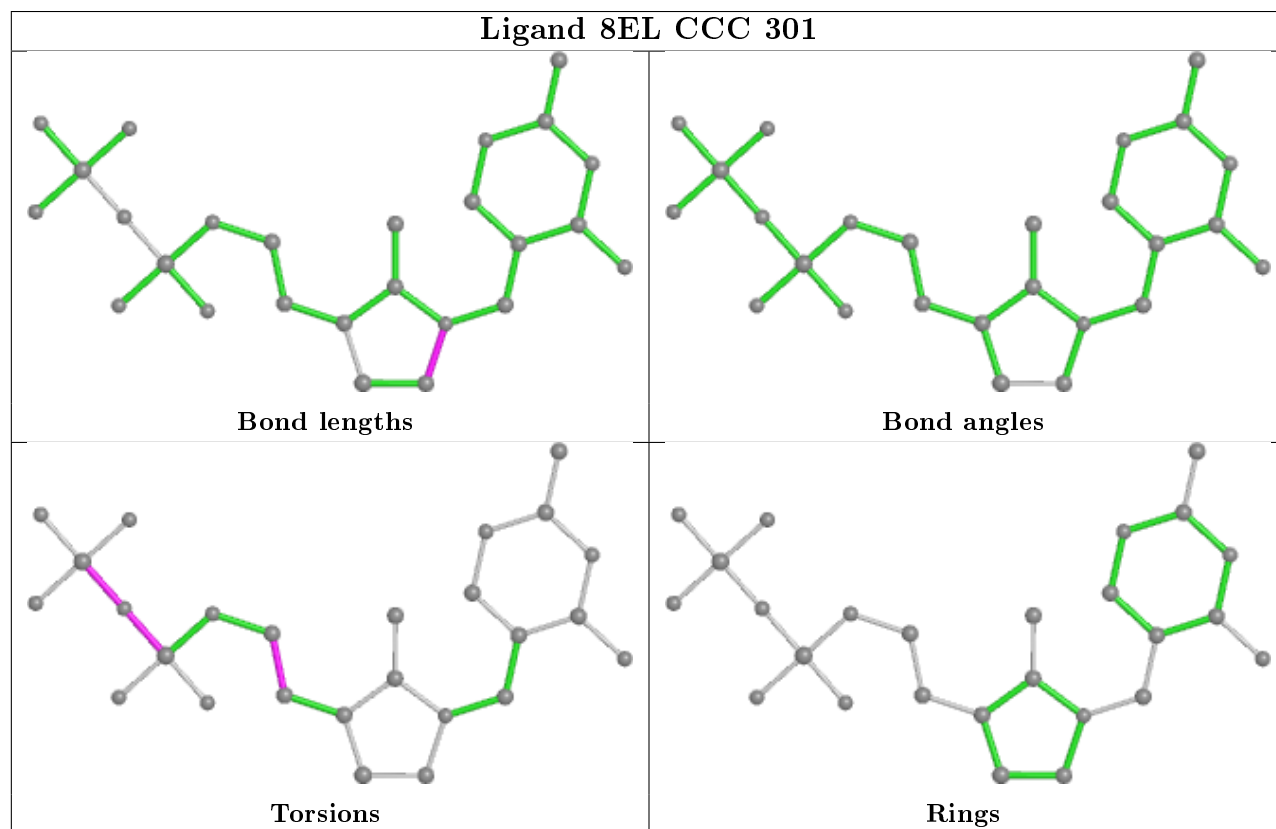
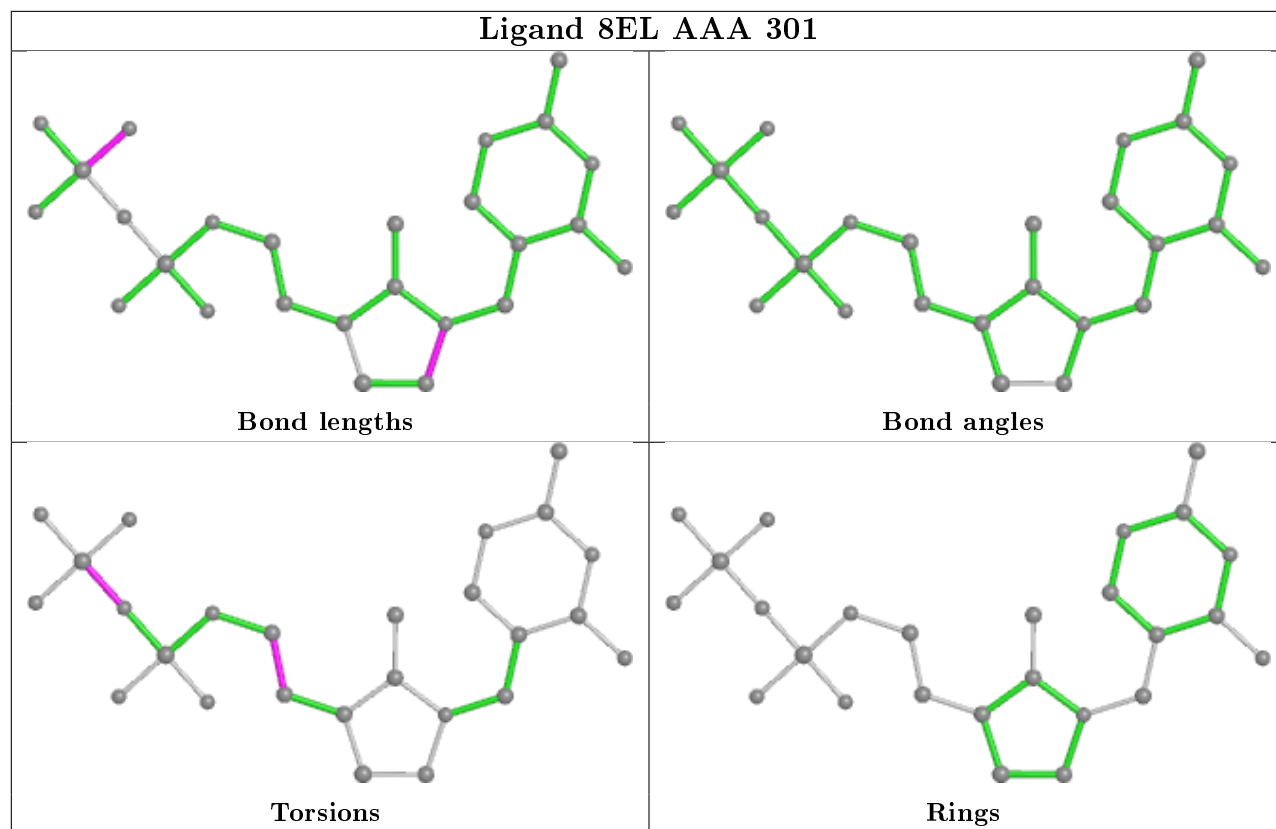
Mol	Chain	Res	Type	Atoms
5	BBB	502	MLT	O3-C2-C3-C4
6	DDD	1401	LMR	C1-C2-C3-C4
6	DDD	1401	LMR	O2-C2-C3-C4
5	CCC	308	MLT	O3-C2-C3-C4
5	CCC	305	MLT	O3-C2-C3-C4
5	AAA	304	MLT	C1-C2-C3-C4
5	AAA	304	MLT	O3-C2-C3-C4
5	CCC	304	MLT	C1-C2-C3-C4
5	CCC	308	MLT	C1-C2-C3-C4
5	CCC	305	MLT	C1-C2-C3-C4
3	CCC	301	8EL	PA-O3A-PB-O1B
3	CCC	301	8EL	PB-O3A-PA-O1A
6	AAA	307	LMR	O2-C2-C3-C4
6	AAA	307	LMR	C1-C2-C3-C4
3	CCC	301	8EL	PB-O3A-PA-O2A
3	AAA	301	8EL	C5-C6-C7-O7
3	CCC	301	8EL	C5-C6-C7-O7

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	502	MLT	1	0
6	AAA	306	LMR	10	0
5	CCC	304	MLT	2	0
6	AAA	307	LMR	1	0
5	BBB	504	MLT	2	0
5	AAA	304	MLT	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.



## 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	AAA	282/309 (91%)	-0.22	8 (2%) 53 59	11, 17, 33, 101	0
1	CCC	282/309 (91%)	-0.06	22 (7%) 13 14	12, 19, 37, 109	0
2	BBB	311/341 (91%)	-0.48	1 (0%) 94 95	11, 15, 27, 70	0
2	DDD	311/341 (91%)	-0.45	1 (0%) 94 95	12, 16, 30, 75	0
All	All	1186/1300 (91%)	-0.31	32 (2%) 54 61	11, 17, 32, 109	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	1	MET	11.4
1	CCC	278[A]	TRP	8.0
1	CCC	-1	ASP	6.8
1	CCC	0	ASP	6.8
1	AAA	1	MET	6.6
1	CCC	2	GLN	6.4
1	AAA	-1	ASP	5.8
1	CCC	280	GLU	5.8
2	DDD	2	GLY	4.8
1	CCC	279	GLU	4.8
1	AAA	278	TRP	4.3
1	AAA	2	GLN	4.3
1	CCC	3[A]	ASP	4.2
2	BBB	2	GLY	4.0
1	AAA	0	ASP	3.7
1	CCC	277	LEU	3.7
1	CCC	272	VAL	3.5
1	AAA	280	GLU	3.3
1	CCC	6	LEU	3.2
1	CCC	275	GLU	3.0
1	CCC	260	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	CCC	261[A]	GLU	2.8
1	AAA	277	LEU	2.8
1	CCC	25[A]	GLU	2.8
1	CCC	263	VAL	2.8
1	CCC	276[A]	LYS	2.7
1	CCC	88[A]	GLU	2.5
1	CCC	5	ILE	2.2
1	CCC	267	LEU	2.2
1	CCC	268[A]	SER	2.1
1	CCC	259	LYS	2.1
1	AAA	279	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MLT	BBB	501	9/9	0.71	0.31	63,79,94,99	1
6	LMR	DDD	1402	9/9	0.72	0.25	46,52,65,65	13
6	LMR	AAA	306	9/9	0.73	0.23	20,23,41,47	13
6	LMR	AAA	308	9/9	0.74	0.23	84,92,100,105	1
6	LMR	AAA	307	9/9	0.74	0.26	50,57,77,77	1
6	LMR	DDD	1401	9/9	0.74	0.28	77,81,111,112	1
5	MLT	BBB	504	9/9	0.75	0.28	30,38,57,67	13
5	MLT	CCC	307	9/9	0.77	0.23	56,64,80,108	1
5	MLT	CCC	304	9/9	0.79	0.30	37,46,55,78	13
5	MLT	AAA	305	9/9	0.79	0.29	59,72,87,97	1
5	MLT	AAA	304	9/9	0.80	0.21	39,57,86,89	1
5	MLT	BBB	502	9/9	0.81	0.33	57,79,88,106	1

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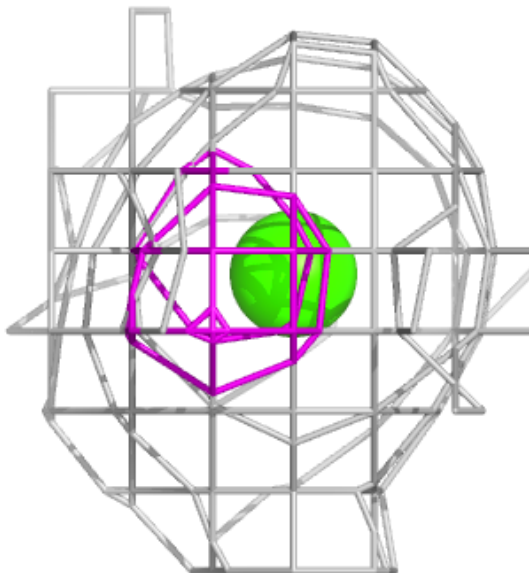
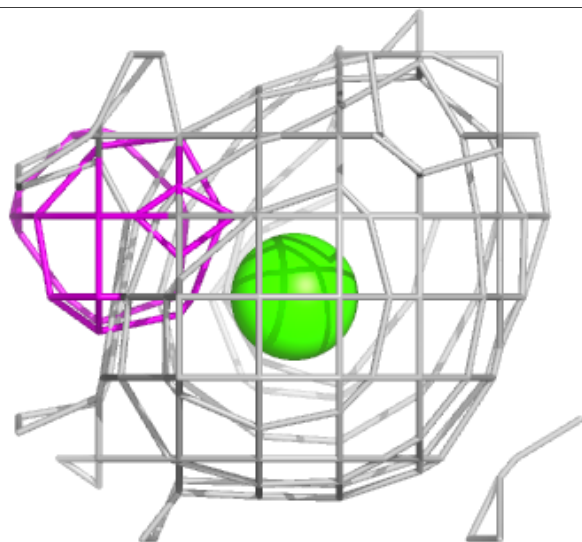
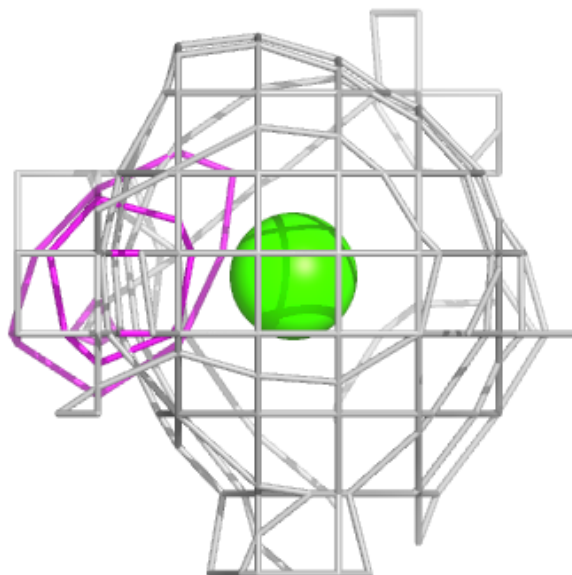
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MLT	CCC	305	9/9	0.82	0.24	43,60,82,82	1
5	MLT	BBB	503	9/9	0.87	0.19	57,72,108,108	1
5	MLT	CCC	308	9/9	0.87	0.22	52,69,75,79	1
5	MLT	CCC	306	9/9	0.88	0.18	31,58,82,82	13
7	CL	DDD	1403	1/1	0.89	0.06	34,34,34,34	1
7	CL	CCC	309	1/1	0.98	0.04	27,27,27,27	0
4	CA	CCC	303	1/1	0.98	0.14	31,31,31,31	1
7	CL	BBB	505	1/1	0.98	0.05	27,27,27,27	0
3	8EL	CCC	301	26/26	0.99	0.04	13,16,20,29	0
4	CA	AAA	303	1/1	0.99	0.06	24,24,24,24	1
3	8EL	AAA	301	26/26	0.99	0.05	13,15,20,29	0
7	CL	AAA	309	1/1	0.99	0.05	24,24,24,24	0
4	CA	AAA	302	1/1	1.00	0.05	13,13,13,13	0
4	CA	CCC	302	1/1	1.00	0.06	14,14,14,14	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.

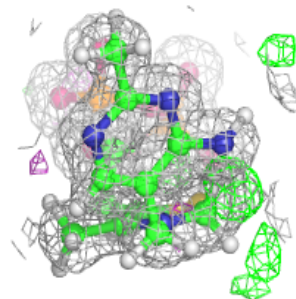
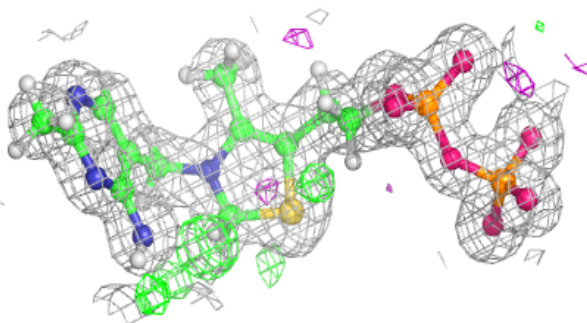
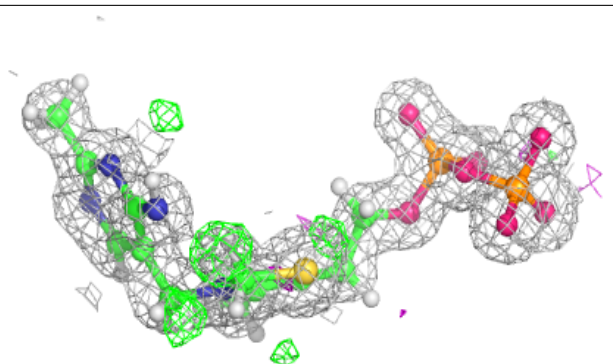
**Electron density around CA CCC 303:**

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



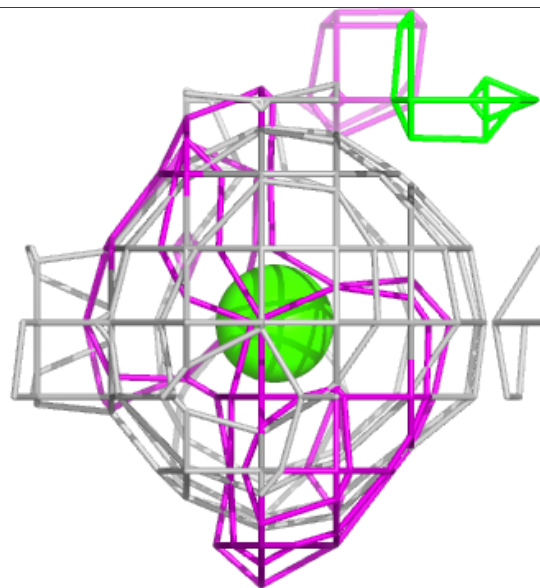
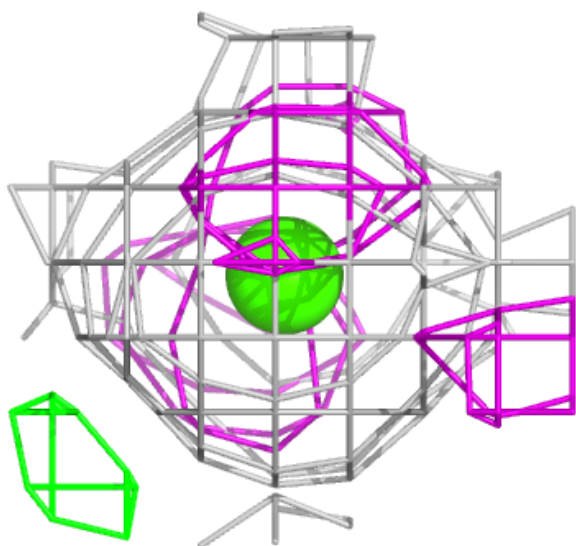
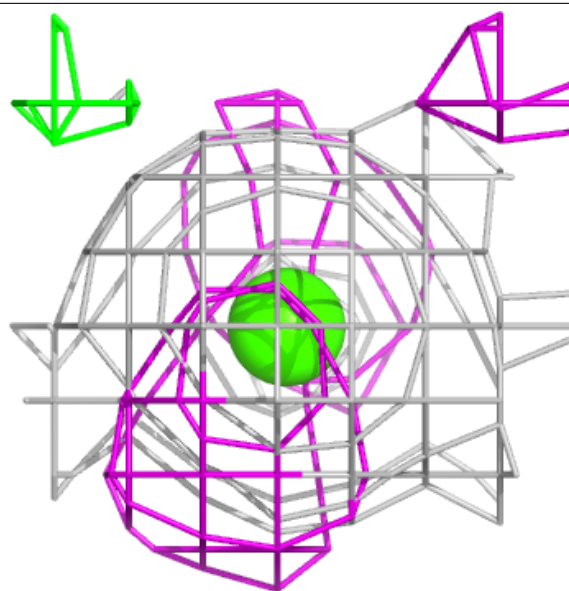
**Electron density around 8EL CCC 301:**

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



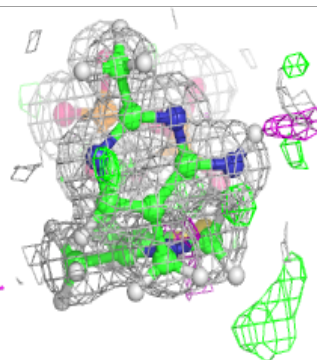
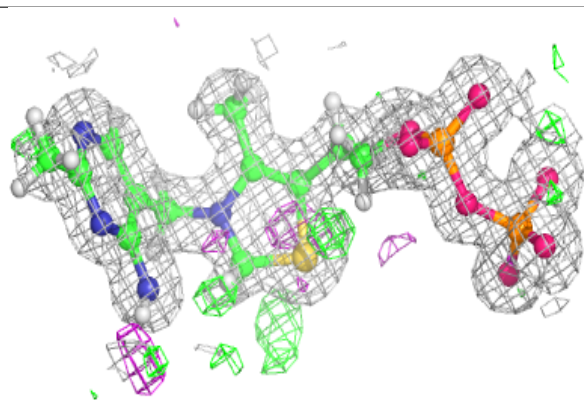
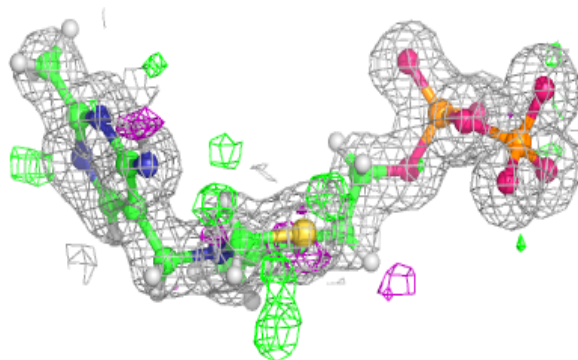
**Electron density around CA AAA 303:**

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



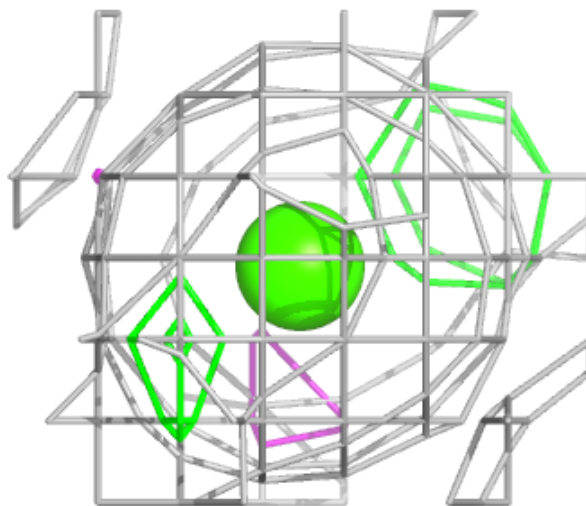
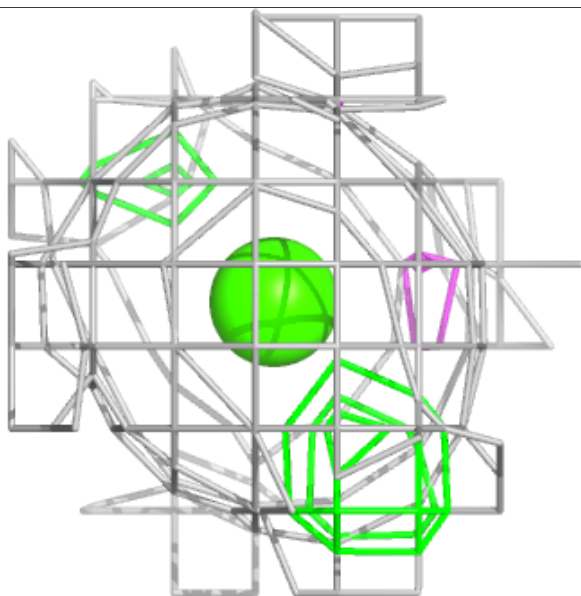
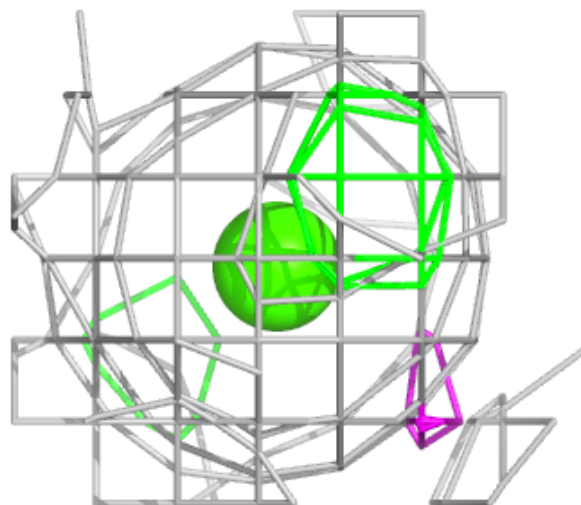
**Electron density around 8EL AAA 301:**

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



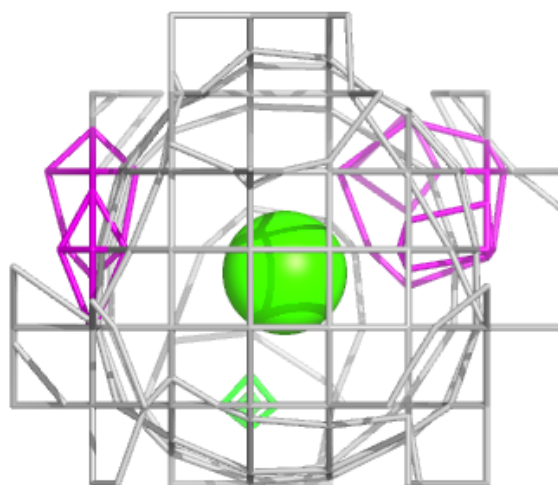
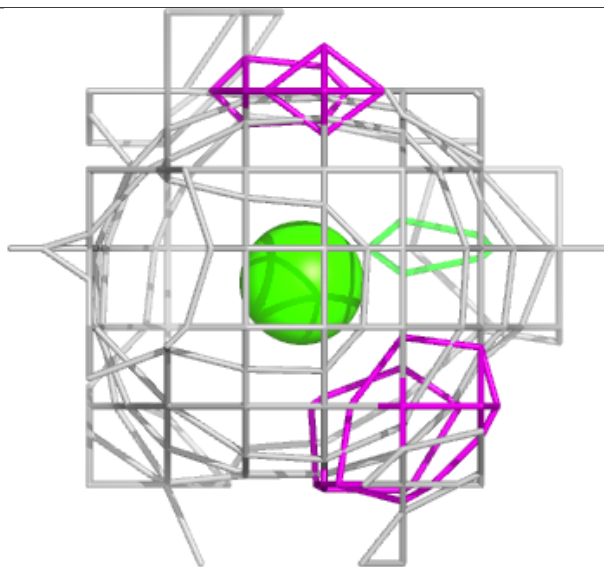
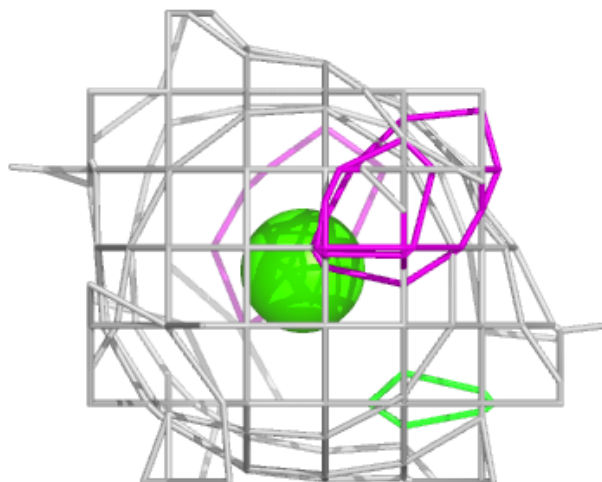
**Electron density around CA AAA 302:**

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



**Electron density around CA CCC 302:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.