



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:12 am BST

PDB ID : 4XHE  
Title : Crystal Structure of A-AChBP in complex with pinnatoxin A  
Authors : Bourne, Y.; Sulzenbacher, G.; Marchot, P.  
Deposited on : 2015-01-05  
Resolution : 1.90 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

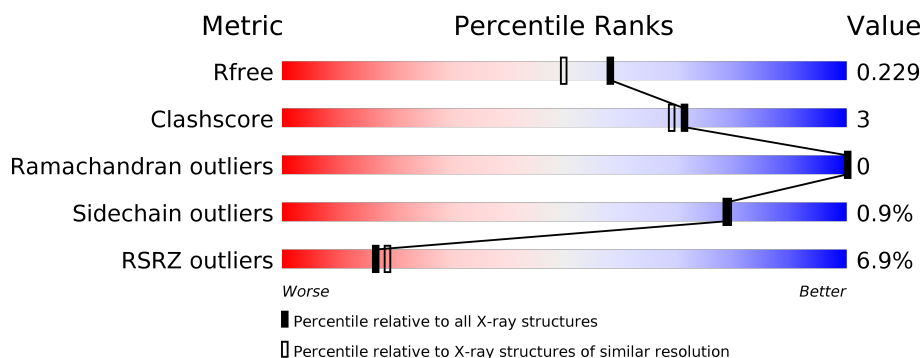
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	217	<div> <div>7%</div> <div>92%</div> <div>8%</div> </div>
1	B	217	<div> <div>6%</div> <div>93%</div> <div>7%</div> </div>
1	C	217	<div> <div>6%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	D	217	<div> <div>7%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
1	E	217	<div> <div>6%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
1	F	217	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	217	<div><div></div><div>8%</div><div>90%</div><div>6%</div><div></div></div>
1	H	217	<div><div></div><div>7%</div><div>90%</div><div>8%</div><div></div></div>
1	I	217	<div><div></div><div>8%</div><div>88%</div><div>6%</div><div>6%</div></div>
1	J	217	<div><div></div><div>6%</div><div>89%</div><div>8%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19628 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	10	0
			1785	1131	294	350	10			
1	B	217	Total	C	N	O	S	0	6	0
			1771	1117	289	354	11			
1	C	211	Total	C	N	O	S	0	8	0
			1720	1091	281	336	12			
1	D	211	Total	C	N	O	S	0	7	0
			1719	1087	285	337	10			
1	E	210	Total	C	N	O	S	0	5	0
			1701	1075	280	336	10			
1	F	213	Total	C	N	O	S	0	7	0
			1735	1096	286	342	11			
1	G	210	Total	C	N	O	S	0	7	0
			1714	1085	281	338	10			
1	H	212	Total	C	N	O	S	0	7	0
			1733	1095	285	342	11			
1	I	204	Total	C	N	O	S	0	7	0
			1671	1061	276	326	8			
1	J	211	Total	C	N	O	S	0	7	0
			1723	1090	281	340	12			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8

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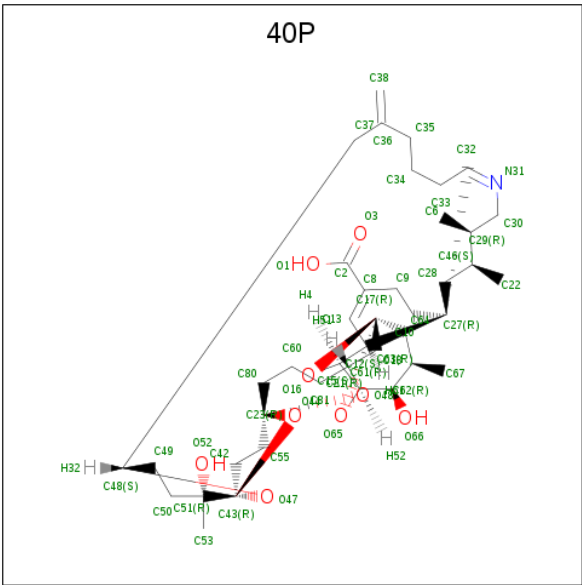
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is Pinnatoxin A (three-letter code: 40P) (formula: C<sub>41</sub>H<sub>61</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	41	1	9		
2	B	1	Total	C	N	O	0	0
			51	41	1	9		
2	C	1	Total	C	N	O	0	0
			51	41	1	9		
2	D	1	Total	C	N	O	0	0
			51	41	1	9		
2	E	1	Total	C	N	O	0	0
			51	41	1	9		
2	F	1	Total	C	N	O	0	0
			51	41	1	9		
2	G	1	Total	C	N	O	0	0
			51	41	1	9		
2	H	1	Total	C	N	O	0	0
			51	41	1	9		
2	I	1	Total	C	N	O	0	0
			51	41	1	9		
2	J	1	Total	C	N	O	0	0
			51	41	1	9		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Ca 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

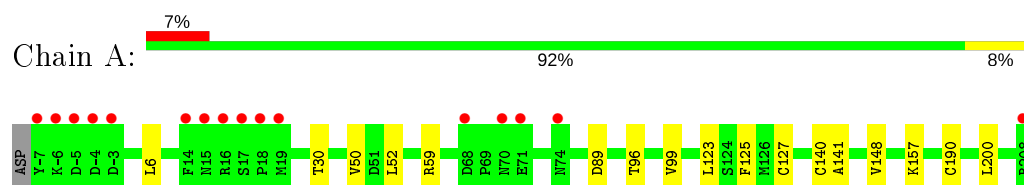
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total 189	O 189	0	0
5	B	180	Total 180	O 180	0	0
5	C	193	Total 193	O 193	0	0
5	D	186	Total 186	O 186	0	0
5	E	182	Total 182	O 182	0	0
5	F	194	Total 194	O 194	0	0
5	G	167	Total 167	O 167	0	0
5	H	188	Total 188	O 188	0	0
5	I	190	Total 190	O 190	0	0
5	J	172	Total 172	O 172	0	0



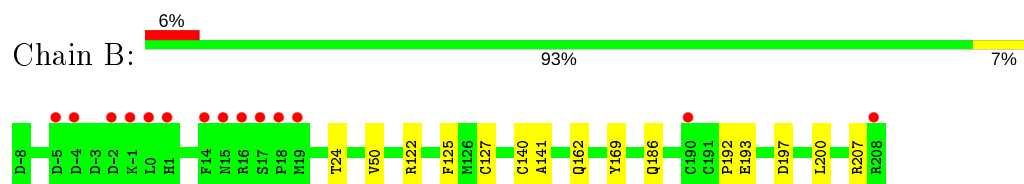
### 3 Residue-property plots [i](#)

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.

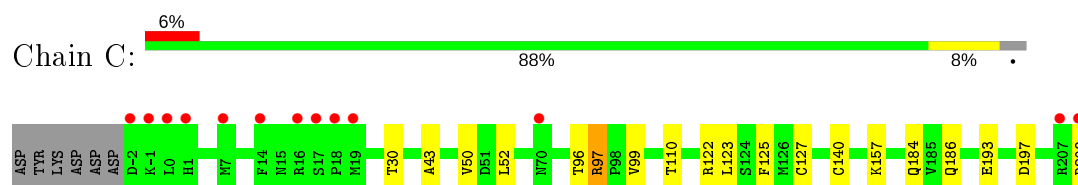
- Molecule 1: Soluble acetylcholine receptor



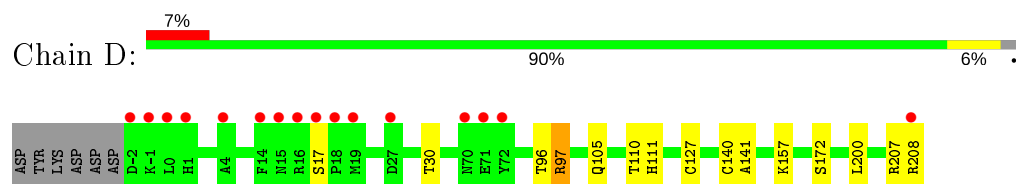
- Molecule 1: Soluble acetylcholine receptor



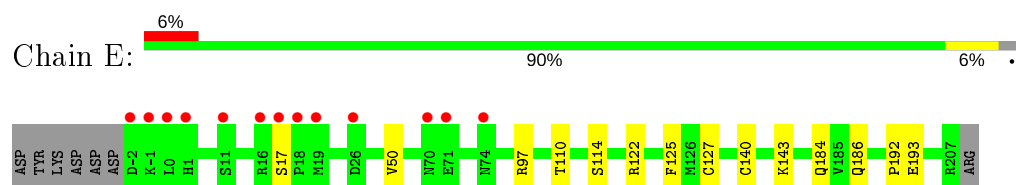
- Molecule 1: Soluble acetylcholine receptor



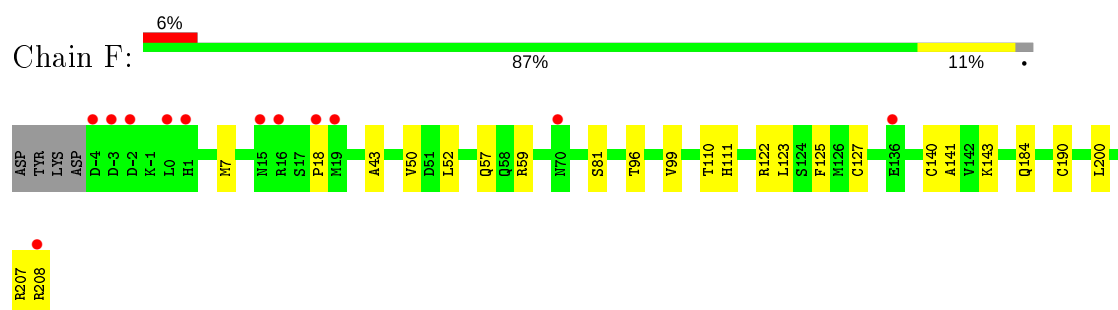
- Molecule 1: Soluble acetylcholine receptor



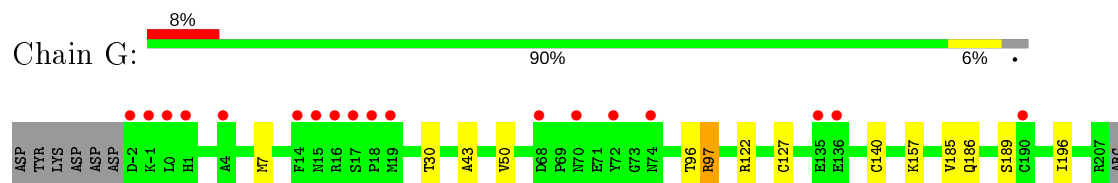
- Molecule 1: Soluble acetylcholine receptor



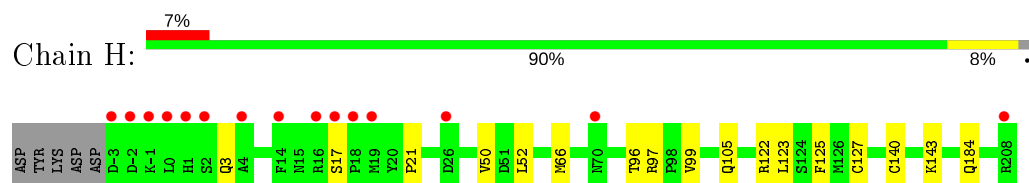
- Molecule 1: Soluble acetylcholine receptor



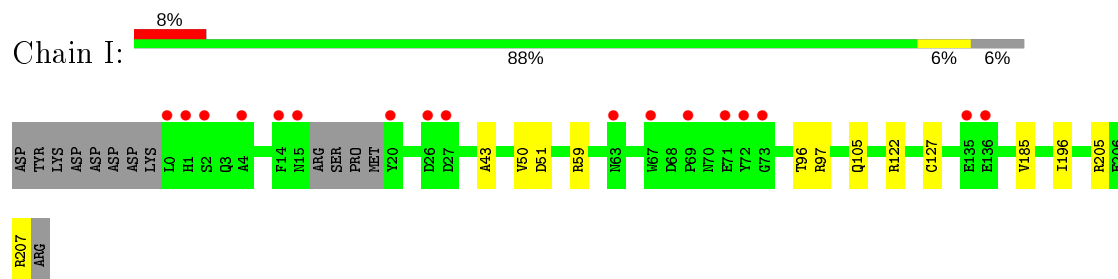
- Molecule 1: Soluble acetylcholine receptor



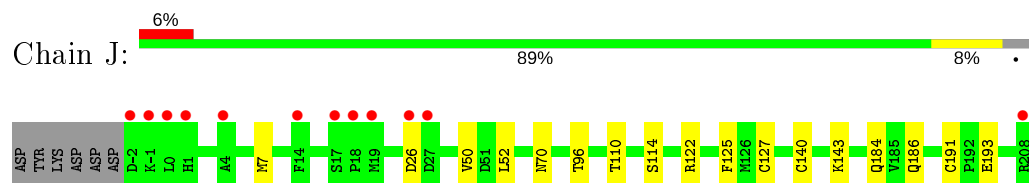
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.73Å 144.23Å 147.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.02 – 1.90 63.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (64.02-1.90) 97.6 (63.99-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.173 , 0.216 0.188 , 0.229	Depositor DCC
$R_{free}$ test set	6419 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9833e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL, 40P

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	0.54	0/1857	0.66	0/2528
1	B	0.53	0/1831	0.66	0/2493
1	C	0.55	0/1785	0.67	0/2432
1	D	0.52	0/1781	0.67	0/2426
1	E	0.52	0/1756	0.67	0/2391
1	F	0.52	0/1797	0.68	0/2447
1	G	0.51	0/1775	0.67	0/2418
1	H	0.50	0/1792	0.66	0/2441
1	I	0.53	0/1730	0.64	1/2355 (0.0%)
1	J	0.53	0/1788	0.66	0/2434
All	All	0.52	0/17892	0.66	1/24365 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	51	ASP	CB-CG-OD1	6.07	123.76	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	CYS	Peptide
1	F	190	CYS	Peptide

## 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	1785	0	1748	13	0
1	B	1771	0	1702	18	0
1	C	1720	0	1683	16	0
1	D	1719	0	1675	9	0
1	E	1701	0	1646	10	0
1	F	1735	0	1686	22	0
1	G	1714	0	1664	9	0
1	H	1733	0	1678	15	0
1	I	1671	0	1630	9	0
1	J	1723	0	1675	12	0
2	A	51	0	60	0	0
2	B	51	0	60	0	0
2	C	51	0	60	0	0
2	D	51	0	60	0	0
2	E	51	0	60	0	0
2	F	51	0	60	0	0
2	G	51	0	60	0	0
2	H	51	0	60	0	0
2	I	51	0	60	0	0
2	J	51	0	60	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	E	1	0	0	0	0
4	J	1	0	0	0	0
5	A	189	0	0	1	0
5	B	180	0	0	2	0
5	C	193	0	0	3	0
5	D	186	0	0	1	0
5	E	182	0	0	2	0
5	F	194	0	0	2	0
5	G	167	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	188	0	0	0	0
5	I	190	0	0	4	0
5	J	172	0	0	1	1
All	All	19628	0	17387	122	1

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 3.

All (122) 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:B:207[B]:ARG:HH11	1:B:207[B]:ARG:HG2	1.22	1.02
1:F:207[A]:ARG:HB3	1:F:207[A]:ARG:HH11	1.28	0.94
1:B:207[B]:ARG:HH11	1:B:207[B]:ARG:CG	1.82	0.92
1:F:207[A]:ARG:CB	1:F:207[A]:ARG:HH11	2.01	0.73
1:E:97[A]:ARG:NH2	5:E:513:HOH:O	2.23	0.70
1:C:127:CYS:SG	1:C:140[B]:CYS:HB3	2.33	0.69
1:H:127:CYS:SG	1:H:140[B]:CYS:HB3	2.31	0.69
1:B:125:PHE:HZ	1:B:140[B]:CYS:HG	1.39	0.69
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.34	0.66
1:G:127:CYS:SG	1:G:140[B]:CYS:HB3	2.36	0.65
1:F:143:LYS:HE2	1:F:184:GLN:HE22	1.62	0.64
1:E:186:GLN:HG3	5:E:559:HOH:O	1.98	0.63
1:F:207[A]:ARG:HB3	1:F:207[A]:ARG:NH1	2.07	0.62
1:A:127:CYS:SG	1:A:140[B]:CYS:HB3	2.39	0.62
1:J:125:PHE:HZ	1:J:140[B]:CYS:HG	1.44	0.62
1:B:207[B]:ARG:NH1	1:B:207[B]:ARG:CG	2.52	0.62
1:E:127:CYS:SG	1:E:140[B]:CYS:HB3	2.40	0.62
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.39	0.61
1:B:207[B]:ARG:NH1	1:B:207[B]:ARG:HG2	2.04	0.60
1:F:59[B]:ARG:NH2	1:F:59[B]:ARG:HB2	2.16	0.60
1:G:185:VAL:HG22	1:G:196:ILE:HD12	1.84	0.60
1:J:143:LYS:HE2	1:J:184:GLN:HE22	1.66	0.59
1:H:143:LYS:HE2	1:H:184:GLN:HE22	1.68	0.58
1:A:125:PHE:HZ	1:A:140[B]:CYS:HG	1.52	0.58
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.44	0.58
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.43	0.58
1:I:59[A]:ARG:NH1	5:I:578:HOH:O	2.23	0.57
1:B:127:CYS:SG	1:B:140[B]:CYS:HB3	2.45	0.57
1:D:127:CYS:SG	1:D:140[B]:CYS:HB3	2.44	0.57
1:J:186:GLN:NE2	5:J:556:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:THR:HG23	1:D:157:LYS:HD2	1.88	0.56
1:C:30:THR:HG23	1:C:157:LYS:HD3	1.87	0.56
1:J:127:CYS:SG	1:J:140[B]:CYS:HB3	2.47	0.55
1:F:57:GLN:NE2	5:F:570:HOH:O	2.40	0.54
1:A:89:ASP:OD2	1:A:148:VAL:HG22	2.07	0.54
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.47	0.54
1:A:96:THR:O	1:E:122:ARG:HD2	2.08	0.53
1:F:96:THR:O	1:J:122:ARG:HD2	2.09	0.52
1:J:50:VAL:CG2	1:J:127:CYS:SG	2.98	0.52
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.49	0.51
1:A:50:VAL:CG2	1:A:127:CYS:SG	2.99	0.51
1:H:125:PHE:HZ	1:H:140[B]:CYS:HG	1.58	0.50
1:C:127:CYS:SG	1:C:140[B]:CYS:CB	2.97	0.50
1:C:110[A]:THR:HG23	5:C:580:HOH:O	2.10	0.50
1:F:59[B]:ARG:HH21	1:F:59[B]:ARG:HB2	1.76	0.50
1:I:207[B]:ARG:NH1	5:I:512:HOH:O	2.44	0.50
1:C:97[B]:ARG:NH1	5:C:503:HOH:O	2.45	0.50
1:C:52:LEU:HG	1:C:125:PHE:HE2	1.77	0.50
1:C:99[A]:VAL:HG22	1:C:123:LEU:HD13	1.94	0.49
1:C:30:THR:CG2	1:C:157:LYS:HD3	2.43	0.49
1:F:99[B]:VAL:HG22	1:F:123:LEU:CD1	2.42	0.49
1:B:192:PRO:HD2	1:B:193[A]:GLU:OE2	2.13	0.48
1:H:99[A]:VAL:HG22	1:H:123:LEU:HD13	1.93	0.48
1:H:105:GLN:HA	1:H:105:GLN:HE21	1.78	0.48
1:F:127:CYS:SG	1:F:140[B]:CYS:HB3	2.52	0.48
1:F:50:VAL:CG2	1:F:127:CYS:SG	3.01	0.48
1:F:18:PRO:HB2	1:J:7:MET:SD	2.53	0.48
1:E:143:LYS:HE2	1:E:184:GLN:HE22	1.79	0.48
1:B:125:PHE:HZ	1:B:140[B]:CYS:SG	2.36	0.48
1:B:186[B]:GLN:NE2	1:B:197:ASP:OD2	2.46	0.48
1:C:193:GLU:HG2	5:C:496:HOH:O	2.13	0.47
1:A:59[A]:ARG:NE	5:A:497:HOH:O	2.37	0.47
1:E:110:THR:OG1	1:E:114[A]:SER:OG	2.31	0.47
1:B:193[A]:GLU:H	1:B:193[A]:GLU:CD	2.19	0.46
1:B:122:ARG:HD2	1:C:96:THR:O	2.15	0.46
1:A:30:THR:HG21	1:A:157[A]:LYS:HD2	1.97	0.46
1:E:125:PHE:HZ	1:E:140[B]:CYS:HG	1.62	0.46
1:G:122:ARG:HD2	1:H:96:THR:O	2.15	0.46
1:C:184:GLN:NE2	1:C:197:ASP:OD2	2.38	0.46
1:F:122:ARG:HD2	1:G:96:THR:O	2.16	0.46
1:I:122:ARG:HD2	1:J:96:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:OH	5:B:472:HOH:O	2.17	0.46
1:F:52:LEU:HG	1:F:125:PHE:HE2	1.81	0.45
1:F:59[B]:ARG:CB	1:F:59[B]:ARG:CZ	2.95	0.45
1:H:122:ARG:HD2	1:I:96:THR:O	2.16	0.45
1:H:99[A]:VAL:HG22	1:H:123:LEU:CD1	2.47	0.44
1:J:110:THR:OG1	1:J:114[A]:SER:OG	2.34	0.44
1:D:97[B]:ARG:NH2	5:D:459:HOH:O	2.51	0.44
1:E:127:CYS:SG	1:E:140[B]:CYS:CB	3.05	0.44
1:F:59[B]:ARG:CB	1:F:59[B]:ARG:NH2	2.80	0.44
1:A:99[A]:VAL:HG22	1:A:123:LEU:HD13	1.99	0.44
1:C:99[A]:VAL:HG22	1:C:123:LEU:CD1	2.48	0.43
1:B:162:GLN:HG3	5:B:483:HOH:O	2.17	0.43
1:G:7:MET:HE2	1:H:21:PRO:HD3	2.01	0.43
1:H:52:LEU:HG	1:H:125:PHE:HE2	1.83	0.43
1:F:110:THR:HG22	1:F:111:HIS:N	2.34	0.43
1:H:105:GLN:HA	1:H:105:GLN:NE2	2.34	0.43
1:A:141:ALA:HA	1:A:200:LEU:O	2.19	0.43
1:B:141:ALA:HA	1:B:200:LEU:O	2.19	0.42
1:F:141:ALA:HA	1:F:200:LEU:O	2.19	0.42
1:J:52:LEU:HG	1:J:125:PHE:HE2	1.84	0.42
1:F:7[A]:MET:HE1	5:F:527:HOH:O	2.19	0.42
1:B:50:VAL:CG2	1:B:127:CYS:SG	3.07	0.42
1:H:50:VAL:CG2	1:H:127:CYS:SG	3.08	0.42
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.59	0.42
1:B:127:CYS:SG	1:B:140[B]:CYS:CB	3.07	0.42
1:C:122:ARG:HD2	1:D:96:THR:O	2.20	0.42
1:F:99[B]:VAL:HG22	1:F:123:LEU:HD13	2.01	0.42
1:H:99[A]:VAL:CG2	1:H:123:LEU:HD13	2.50	0.42
1:D:110:THR:HG22	1:D:111:HIS:N	2.35	0.42
1:D:141:ALA:HA	1:D:200:LEU:O	2.20	0.42
1:A:99[A]:VAL:HG22	1:A:123:LEU:CD1	2.50	0.41
1:H:3:GLN:HG2	5:I:534:HOH:O	2.20	0.41
1:D:172:SER:O	1:D:207[B]:ARG:NE	2.52	0.41
1:I:185:VAL:HG22	1:I:196:ILE:HD12	2.01	0.41
1:C:43:ALA:HA	1:C:50[A]:VAL:HG22	2.02	0.41
1:C:50[B]:VAL:HG22	1:C:127:CYS:HB3	2.02	0.41
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.60	0.41
1:A:6:LEU:HD22	1:B:24:THR:CG2	2.51	0.41
1:G:30:THR:CG2	1:G:157:LYS:HE2	2.50	0.41
1:A:52:LEU:HG	1:A:125:PHE:HE2	1.86	0.41
1:G:43:ALA:HA	1:G:50:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:GLN:HA	1:D:105:GLN:NE2	2.36	0.41
1:D:30:THR:CG2	1:D:157:LYS:HD2	2.50	0.41
1:I:105:GLN:HE21	1:I:105:GLN:HA	1.86	0.41
1:I:43:ALA:HA	1:I:50:VAL:HG22	2.03	0.40
1:I:97[B]:ARG:NH2	5:I:574:HOH:O	2.54	0.40
1:C:50[B]:VAL:HG11	1:C:127:CYS:SG	2.61	0.40
1:E:192:PRO:HD2	1:E:193:GLU:OE2	2.22	0.40
1:G:97[B]:ARG:NH1	5:G:472:HOH:O	2.54	0.40
1:F:43:ALA:HA	1:F:50:VAL:HG22	2.03	0.40
1:J:191:CYS:HB3	1:J:193[B]:GLU:OE1	2.21	0.40

All (1) 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)
5:G:411:HOH:O	5:J:407:HOH:O[3_445]	2.18	0.02

## 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	224/217 (103%)	222 (99%)	2 (1%)	0	100	100
1	B	221/217 (102%)	216 (98%)	5 (2%)	0	100	100
1	C	217/217 (100%)	216 (100%)	1 (0%)	0	100	100
1	D	216/217 (100%)	214 (99%)	2 (1%)	0	100	100
1	E	212/217 (98%)	209 (99%)	3 (1%)	0	100	100
1	F	218/217 (100%)	213 (98%)	5 (2%)	0	100	100
1	G	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
1	H	217/217 (100%)	216 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	206/217 (95%)	202 (98%)	4 (2%)	0	100	100
1	J	217/217 (100%)	215 (99%)	2 (1%)	0	100	100
All	All	2162/2170 (100%)	2134 (99%)	28 (1%)	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	A	207/198 (104%)	207 (100%)	0	100	100
1	B	204/198 (103%)	204 (100%)	0	100	100
1	C	200/198 (101%)	196 (98%)	4 (2%)	55	51
1	D	199/198 (100%)	195 (98%)	4 (2%)	55	51
1	E	196/198 (99%)	195 (100%)	1 (0%)	88	89
1	F	201/198 (102%)	199 (99%)	2 (1%)	76	76
1	G	198/198 (100%)	193 (98%)	5 (2%)	47	41
1	H	200/198 (101%)	196 (98%)	4 (2%)	55	51
1	I	192/198 (97%)	190 (99%)	2 (1%)	76	76
1	J	200/198 (101%)	198 (99%)	2 (1%)	76	76
All	All	1997/1980 (101%)	1973 (99%)	24 (1%)	78	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	97[A]	ARG
1	C	97[B]	ARG
1	C	186	GLN
1	C	208	ARG
1	D	17	SER
1	D	97[A]	ARG

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Mol	Chain	Res	Type
1	D	97[B]	ARG
1	D	208	ARG
1	E	17	SER
1	F	81	SER
1	F	208	ARG
1	G	97[A]	ARG
1	G	97[B]	ARG
1	G	186[A]	GLN
1	G	186[B]	GLN
1	G	189	SER
1	H	17	SER
1	H	66	MET
1	H	97[A]	ARG
1	H	97[B]	ARG
1	I	205[A]	ARG
1	I	205[B]	ARG
1	J	26	ASP
1	J	70	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	B	74	ASN
1	B	162	GLN
1	C	15	ASN
1	D	15	ASN
1	D	105	GLN
1	E	105	GLN
1	F	184	GLN
1	G	105	GLN
1	H	105	GLN
1	H	184	GLN
1	I	105	GLN
1	J	184	GLN
1	J	186	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
2	40P	F	301	-	50,58,58	0.81	2 (4%)	48,93,93	1.87	13 (27%)
2	40P	E	301	-	50,58,58	0.88	1 (2%)	48,93,93	1.92	12 (25%)
2	40P	D	301	-	50,58,58	0.75	0	48,93,93	1.67	10 (20%)
2	40P	C	301	-	50,58,58	0.61	0	48,93,93	1.76	13 (27%)
2	40P	B	301	-	50,58,58	0.79	0	48,93,93	1.83	11 (22%)
2	40P	A	301	-	50,58,58	0.79	0	48,93,93	1.93	13 (27%)
2	40P	J	301	-	50,58,58	0.83	0	48,93,93	1.91	12 (25%)
2	40P	I	301	-	50,58,58	0.73	0	48,93,93	1.58	9 (18%)
2	40P	H	301	-	50,58,58	0.68	0	48,93,93	1.76	12 (25%)
2	40P	G	301	-	50,58,58	0.81	0	48,93,93	1.73	9 (18%)

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	40P	F	301	-	-	0/16/131/131	-
2	40P	E	301	-	-	1/16/131/131	-
2	40P	D	301	-	-	0/16/131/131	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	40P	C	301	-	-	0/16/131/131	-
2	40P	B	301	-	-	0/16/131/131	-
2	40P	A	301	-	-	0/16/131/131	-
2	40P	J	301	-	-	0/16/131/131	-
2	40P	I	301	-	-	0/16/131/131	-
2	40P	H	301	-	-	0/16/131/131	-
2	40P	G	301	-	-	0/16/131/131	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	40P	C30-N31	2.29	1.49	1.46
2	F	301	40P	C29-C46	-2.07	1.51	1.54
2	F	301	40P	C64-C17	2.01	1.55	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	301	40P	O47-C48-C37	6.56	112.05	105.78
2	A	301	40P	C60-C80-C23	-5.75	104.04	111.53
2	D	301	40P	O48-C21-C81	-5.20	103.52	110.10
2	A	301	40P	O48-C21-C81	-5.17	103.55	110.10
2	F	301	40P	O48-C21-C81	-5.03	103.73	110.10
2	J	301	40P	O16-C15-C12	4.99	115.23	109.07
2	E	301	40P	O47-C48-C37	4.80	110.37	105.78
2	H	301	40P	O16-C15-C12	4.76	114.95	109.07
2	E	301	40P	C42-C55-C23	4.71	108.43	103.14
2	G	301	40P	O47-C48-C37	4.68	110.25	105.78
2	E	301	40P	C60-C80-C23	-4.64	105.48	111.53
2	E	301	40P	O48-C21-C81	-4.57	104.31	110.10
2	G	301	40P	O16-C15-C12	4.57	114.71	109.07
2	B	301	40P	O16-C15-C12	4.56	114.71	109.07
2	I	301	40P	O48-C21-C81	-4.48	104.43	110.10
2	C	301	40P	O16-C15-C12	4.47	114.59	109.07
2	B	301	40P	O47-C48-C37	4.40	109.98	105.78
2	J	301	40P	O48-C21-C81	-4.34	104.61	110.10
2	I	301	40P	C60-C80-C23	-4.27	105.97	111.53
2	F	301	40P	C60-C80-C23	-4.14	106.14	111.53
2	E	301	40P	O16-C17-C18	4.10	115.75	109.45
2	E	301	40P	O16-C15-C12	4.09	114.11	109.07
2	B	301	40P	O48-C21-C81	-4.04	104.98	110.10
2	B	301	40P	C60-C80-C23	-4.04	106.27	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	40P	O16-C17-C18	4.03	115.65	109.45
2	H	301	40P	O16-C17-C18	3.90	115.44	109.45
2	F	301	40P	O47-C48-C49	3.81	114.92	110.10
2	F	301	40P	O16-C15-C12	3.80	113.76	109.07
2	D	301	40P	O47-C48-C37	3.79	109.40	105.78
2	A	301	40P	O47-C48-C37	3.77	109.39	105.78
2	G	301	40P	O48-C21-C18	-3.76	96.48	106.97
2	A	301	40P	O48-C21-C18	-3.75	96.52	106.97
2	B	301	40P	O48-C21-C18	-3.73	96.56	106.97
2	D	301	40P	C42-C55-C23	3.70	107.30	103.14
2	C	301	40P	C42-C55-C23	3.65	107.25	103.14
2	D	301	40P	O48-C21-C18	-3.60	96.93	106.97
2	C	301	40P	O48-C21-C18	-3.58	96.98	106.97
2	F	301	40P	C42-C55-C23	3.54	107.11	103.14
2	A	301	40P	O16-C15-C12	3.53	113.43	109.07
2	A	301	40P	C42-C55-C23	3.48	107.05	103.14
2	I	301	40P	C42-C55-C23	3.47	107.04	103.14
2	B	301	40P	C17-O65-C61	-3.42	101.81	107.47
2	D	301	40P	C60-C80-C23	-3.33	107.20	111.53
2	G	301	40P	C17-O65-C61	-3.29	102.03	107.47
2	I	301	40P	O48-C21-C18	-3.29	97.81	106.97
2	J	301	40P	O48-C21-C18	-3.26	97.90	106.97
2	F	301	40P	O48-C21-C18	-3.25	97.91	106.97
2	C	301	40P	O47-C48-C37	3.23	108.87	105.78
2	C	301	40P	O44-C43-C42	3.18	107.69	104.64
2	B	301	40P	O44-C43-C42	3.15	107.67	104.64
2	H	301	40P	C60-C80-C23	-3.15	107.43	111.53
2	A	301	40P	O16-C17-C18	3.12	114.25	109.45
2	G	301	40P	C60-C80-C23	-3.07	107.53	111.53
2	H	301	40P	O48-C21-C18	-3.07	98.40	106.97
2	H	301	40P	O47-C48-C37	3.07	108.71	105.78
2	D	301	40P	O47-C43-C51	-3.05	106.79	110.21
2	J	301	40P	C60-C80-C23	-3.03	107.58	111.53
2	G	301	40P	C42-C55-C23	3.03	106.54	103.14
2	C	301	40P	O47-C43-C51	-3.02	106.83	110.21
2	J	301	40P	O16-C17-C18	2.96	114.00	109.45
2	H	301	40P	C42-C55-C23	2.85	106.34	103.14
2	H	301	40P	O47-C48-C49	2.85	113.70	110.10
2	C	301	40P	O16-C17-C18	2.82	113.79	109.45
2	G	301	40P	O47-C43-C51	-2.82	107.06	110.21
2	A	301	40P	O44-C43-C42	2.81	107.34	104.64
2	B	301	40P	C42-C55-C23	2.79	106.27	103.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	40P	O16-C15-C12	2.78	112.50	109.07
2	J	301	40P	C17-O65-C61	-2.72	102.96	107.47
2	F	301	40P	O47-C48-C37	2.69	108.35	105.78
2	I	301	40P	C17-O65-C61	-2.65	103.09	107.47
2	H	301	40P	O48-C21-C81	-2.63	106.77	110.10
2	D	301	40P	O16-C17-C18	2.57	113.41	109.45
2	I	301	40P	O47-C48-C49	2.57	113.36	110.10
2	E	301	40P	O48-C21-C18	-2.57	99.80	106.97
2	A	301	40P	O44-C23-C55	2.57	107.48	104.90
2	C	301	40P	C80-C60-C81	2.50	115.45	111.38
2	C	301	40P	O48-C21-C81	-2.49	106.94	110.10
2	B	301	40P	O16-C17-C18	2.48	113.27	109.45
2	C	301	40P	C60-C80-C23	-2.46	108.33	111.53
2	E	301	40P	O52-C51-C43	2.46	112.51	107.56
2	I	301	40P	O47-C48-C37	2.45	108.12	105.78
2	F	301	40P	O44-C43-C42	2.44	106.98	104.64
2	D	301	40P	C17-O65-C61	-2.43	103.45	107.47
2	J	301	40P	C42-C55-C23	2.42	105.86	103.14
2	B	301	40P	O47-C48-C49	2.41	113.16	110.10
2	J	301	40P	O47-C43-C51	-2.41	107.51	110.21
2	F	301	40P	O16-C17-C18	2.37	113.09	109.45
2	C	301	40P	C17-O65-C61	-2.36	103.56	107.47
2	I	301	40P	O16-C17-C18	2.30	112.99	109.45
2	F	301	40P	O66-C62-C63	-2.30	107.44	110.61
2	C	301	40P	O44-C23-C55	2.29	107.21	104.90
2	H	301	40P	O66-C62-C63	-2.29	107.46	110.61
2	H	301	40P	O65-C17-O16	-2.28	103.42	105.55
2	F	301	40P	C17-O65-C61	-2.28	103.70	107.47
2	B	301	40P	O47-C43-C51	-2.27	107.67	110.21
2	E	301	40P	O65-C61-C15	-2.22	100.05	103.58
2	D	301	40P	O16-C15-C12	2.19	111.78	109.07
2	H	301	40P	O47-C43-C51	-2.19	107.75	110.21
2	A	301	40P	C17-O65-C61	-2.19	103.84	107.47
2	F	301	40P	O65-C61-C15	-2.17	100.11	103.58
2	J	301	40P	C67-C63-C62	2.17	115.38	112.44
2	J	301	40P	O44-C23-C55	2.13	107.05	104.90
2	F	301	40P	O65-C17-O16	-2.13	103.56	105.55
2	C	301	40P	C60-C81-C21	2.13	115.73	110.62
2	A	301	40P	C18-C21-C81	2.12	120.75	112.68
2	E	301	40P	C49-C50-C51	-2.12	111.02	113.25
2	A	301	40P	O65-C61-C15	-2.09	100.25	103.58
2	A	301	40P	O47-C48-C49	2.09	112.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	40P	C28-C46-C29	-2.07	109.91	114.43
2	E	301	40P	O66-C62-C61	-2.05	104.50	109.94
2	G	301	40P	O44-C43-C42	2.04	106.60	104.64
2	D	301	40P	O65-C61-C15	-2.03	100.35	103.58
2	J	301	40P	C50-C49-C48	2.01	113.75	110.33
2	H	301	40P	O44-C23-C55	2.01	106.92	104.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	40P	O16-C17-C18-C21

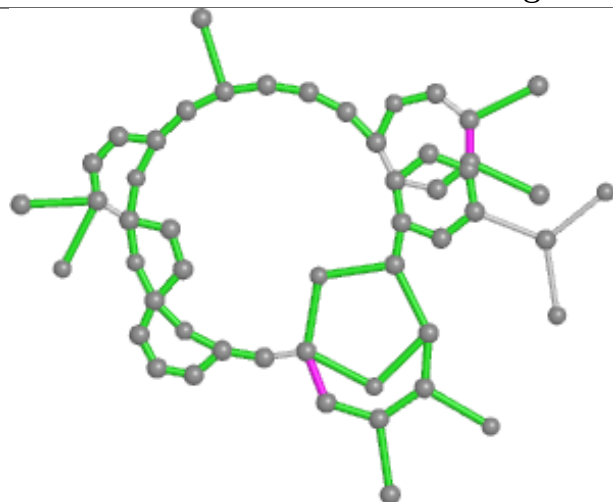
There are no ring outliers.

No monomer is involved in short contacts.

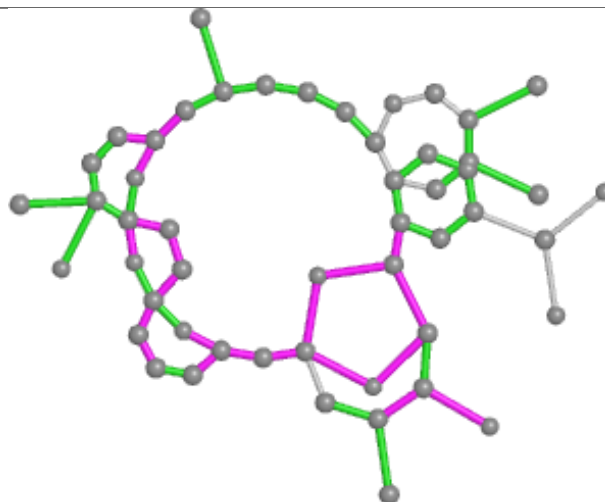
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



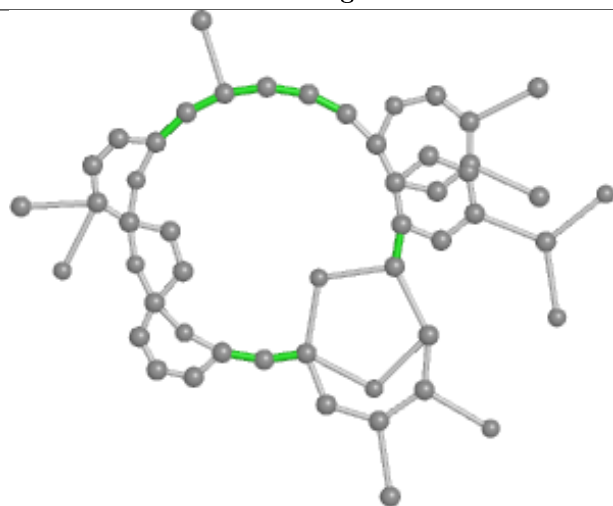
## Ligand 40P F 301



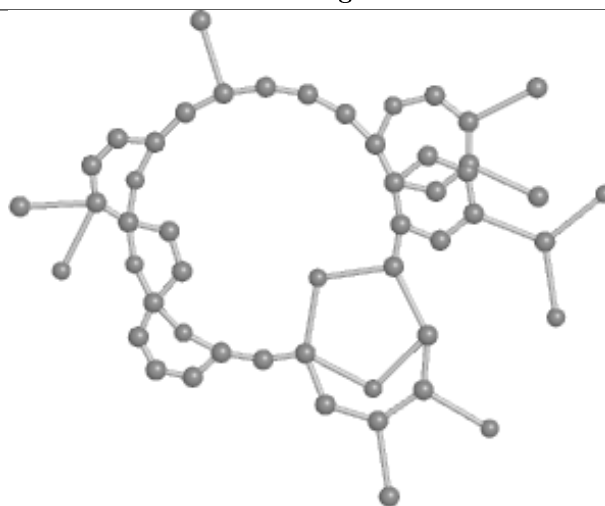
Bond lengths



Bond angles

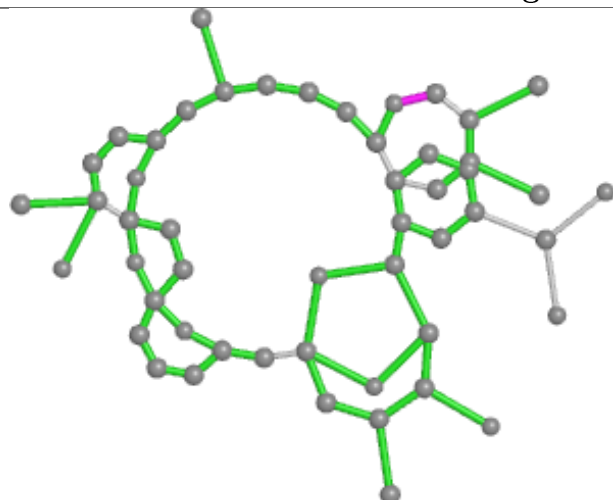


Torsions

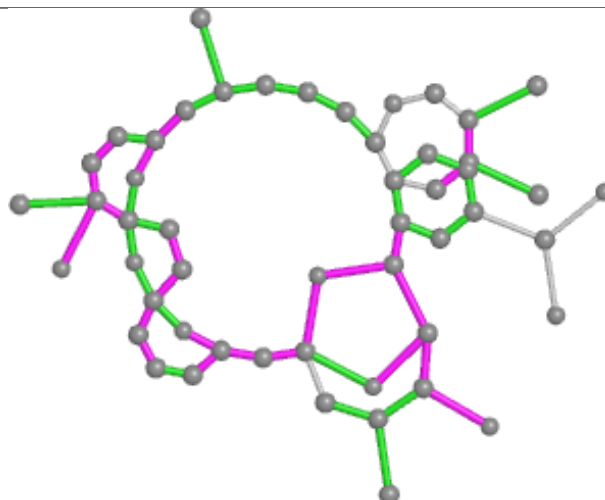


Rings

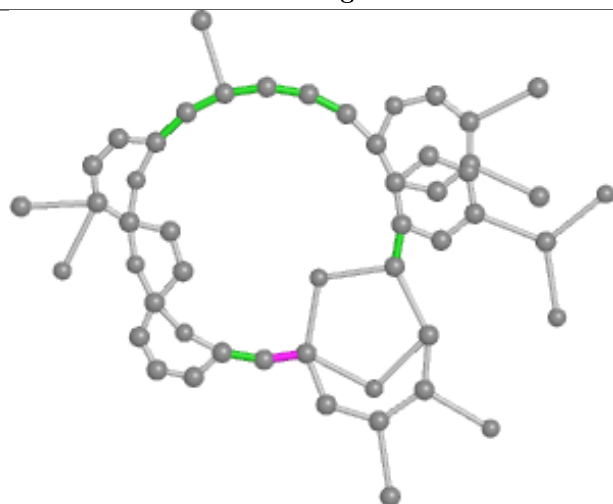
## Ligand 40P E 301



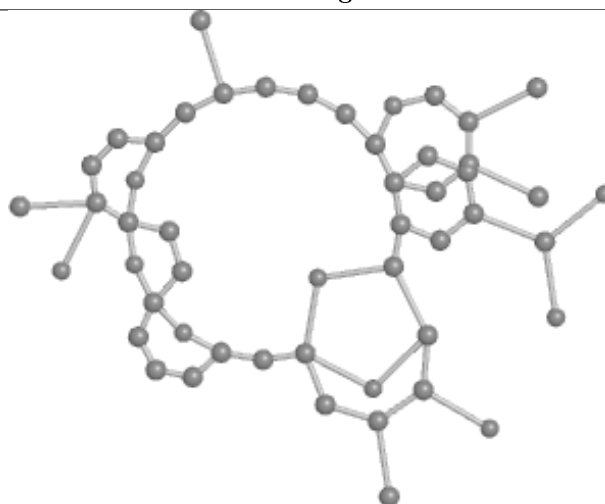
Bond lengths



Bond angles

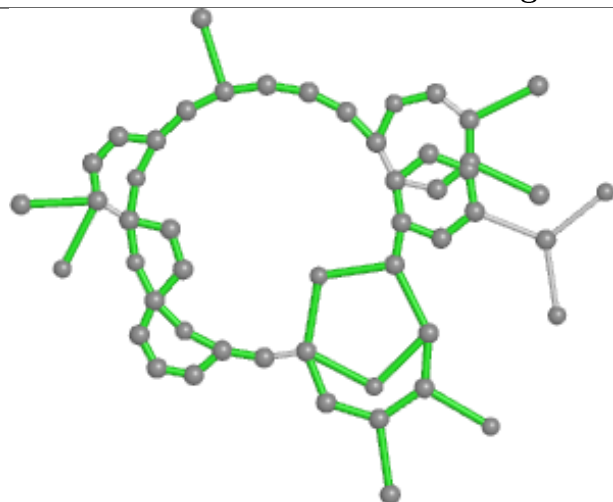


Torsions

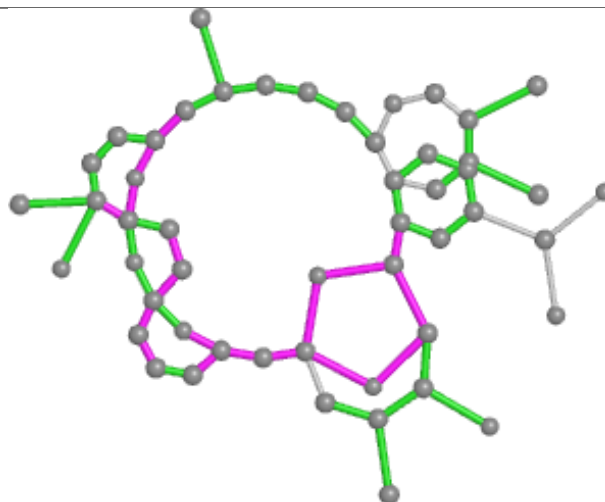


Rings

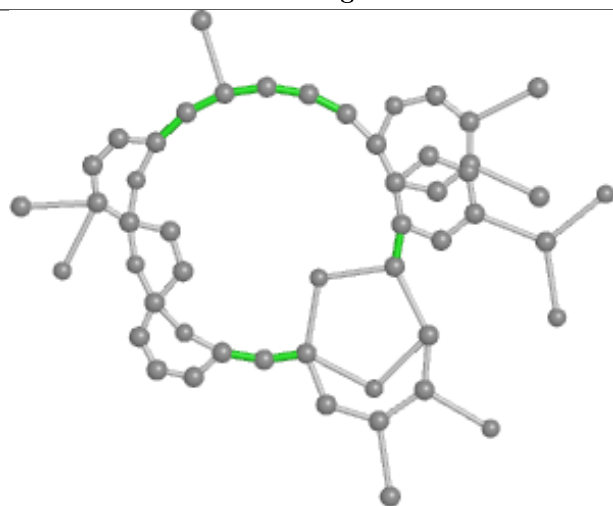
## Ligand 40P D 301



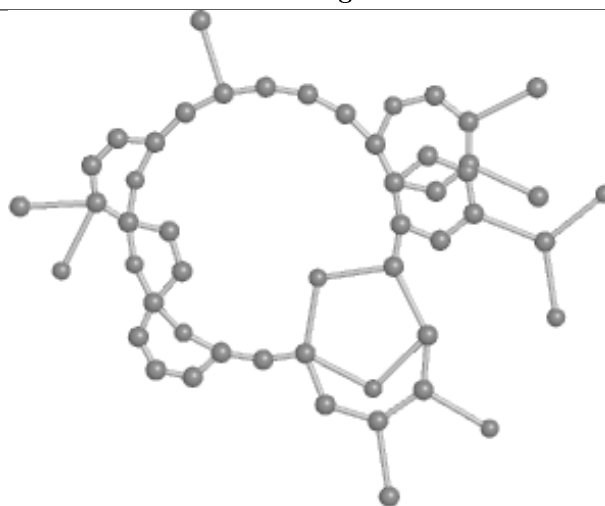
Bond lengths



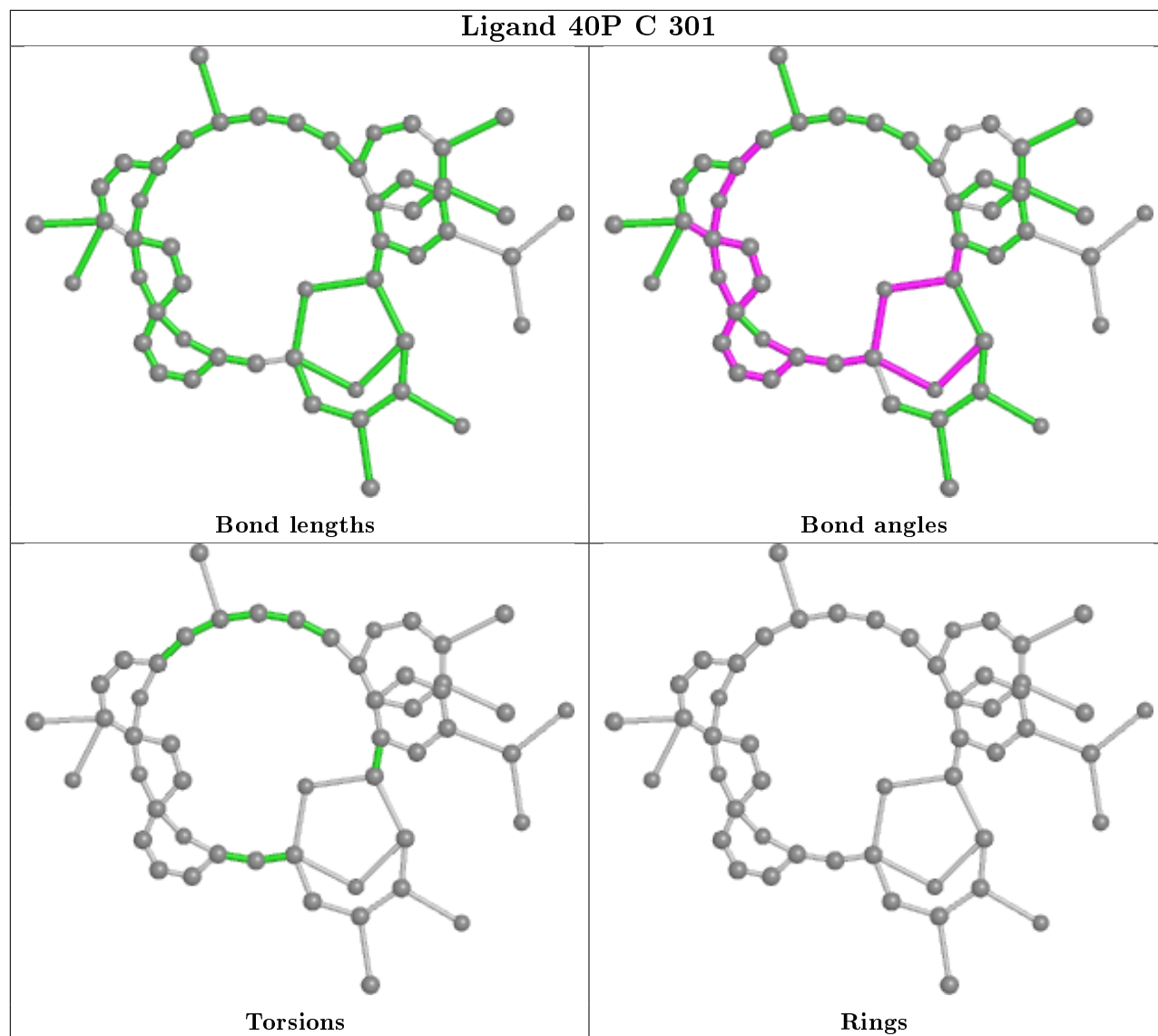
Bond angles



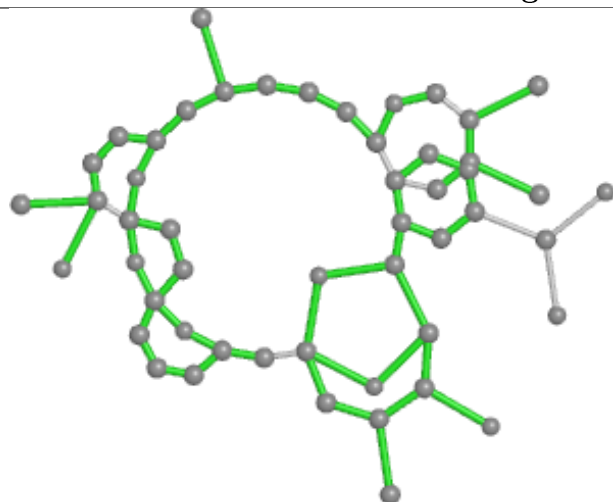
Torsions



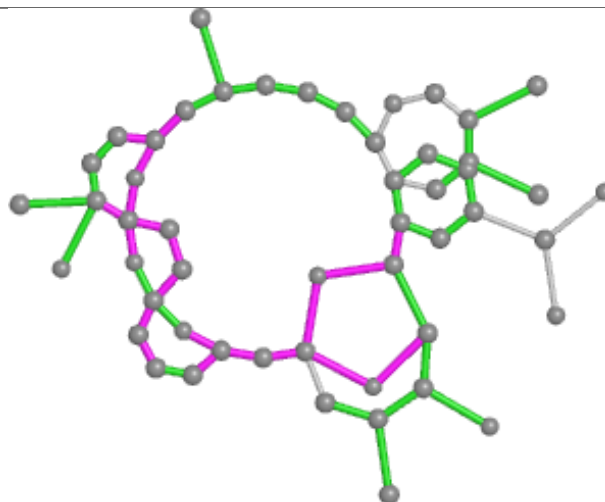
Rings



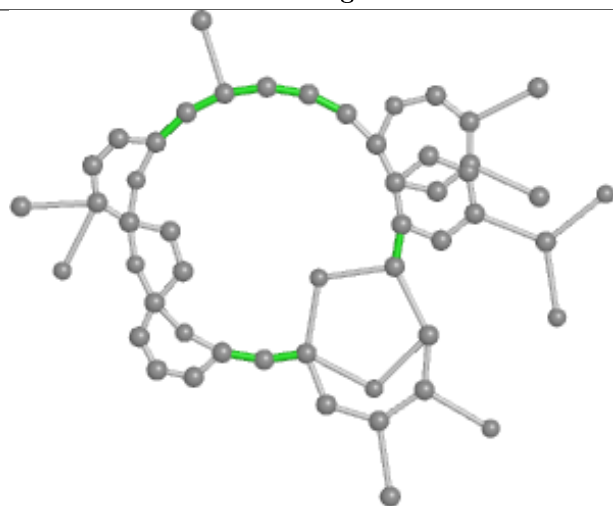
## Ligand 40P B 301



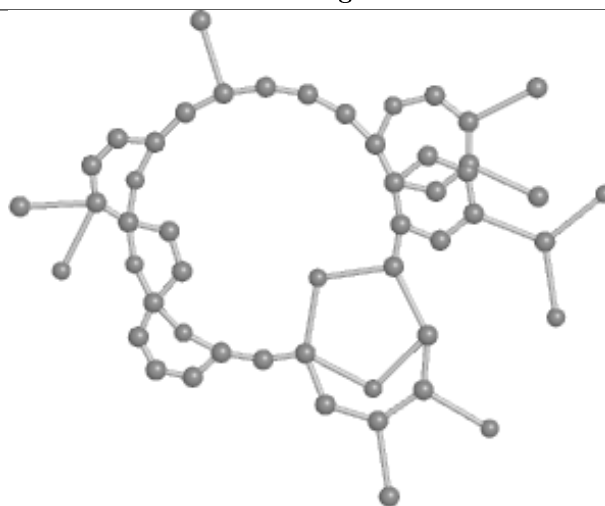
Bond lengths



Bond angles

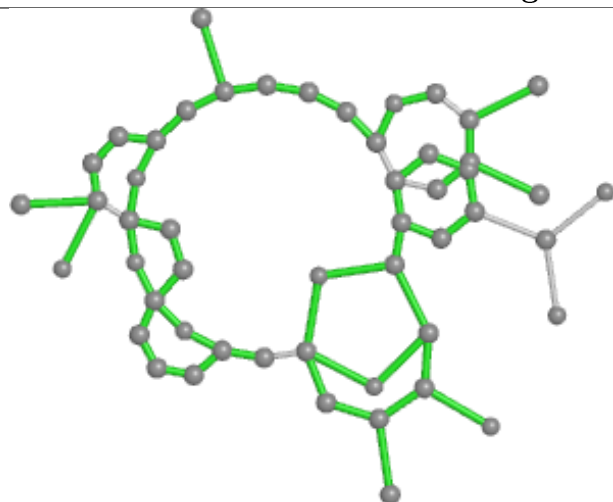


Torsions

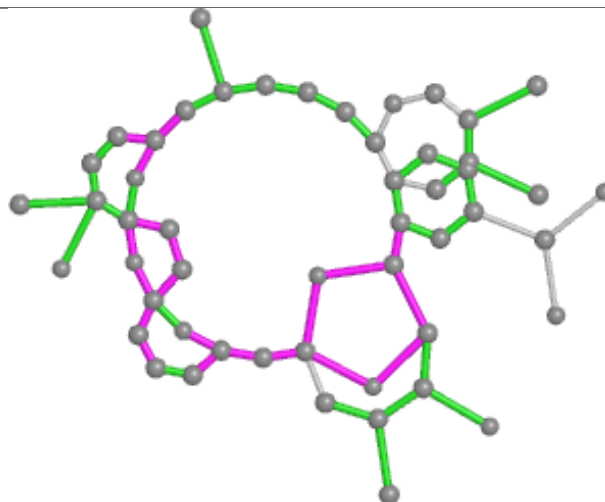


Rings

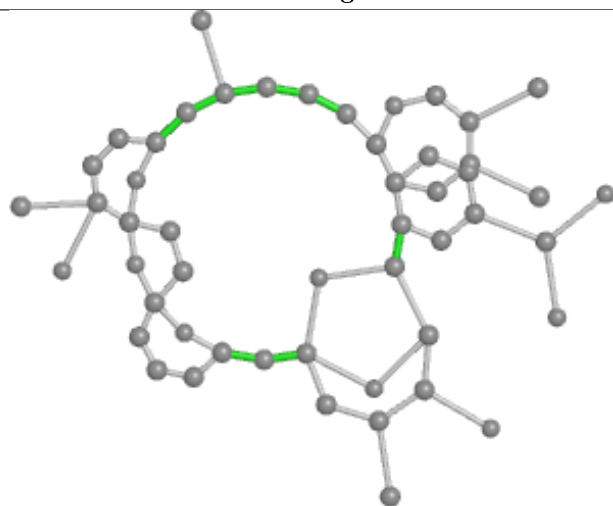
## Ligand 40P A 301



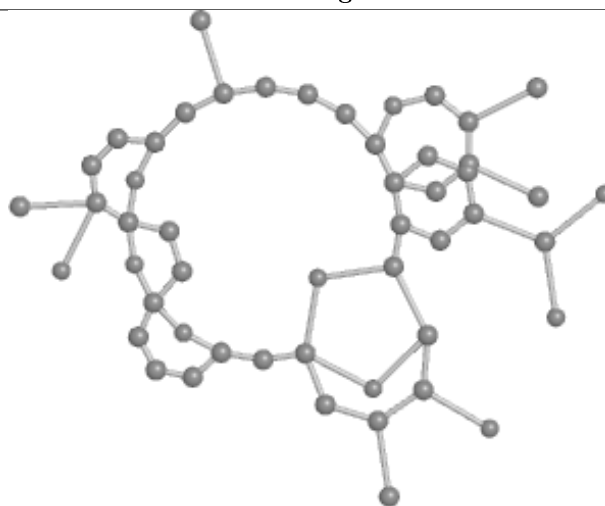
Bond lengths



Bond angles

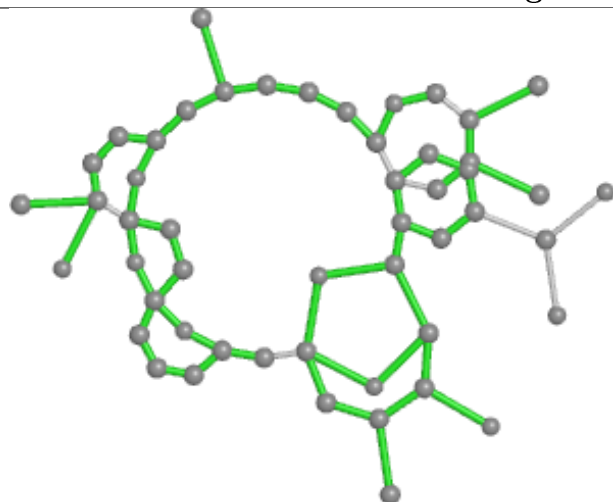


Torsions

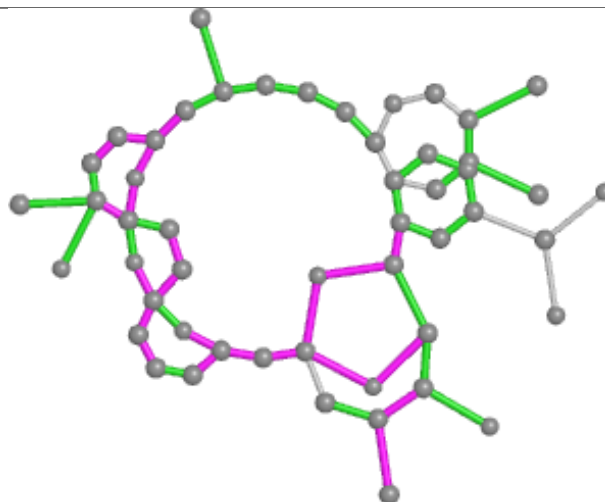


Rings

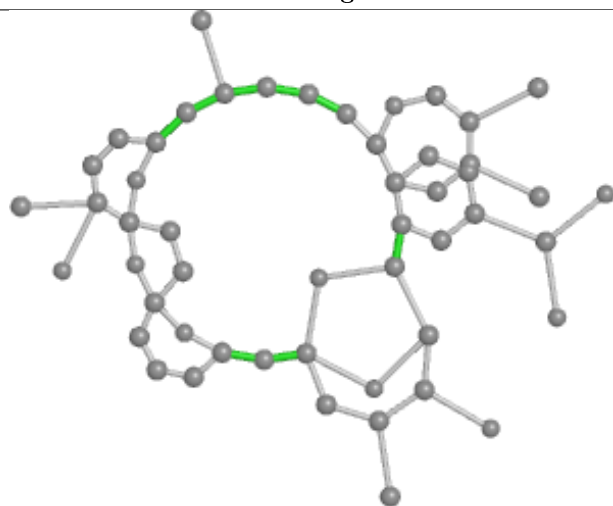
## Ligand 40P J 301



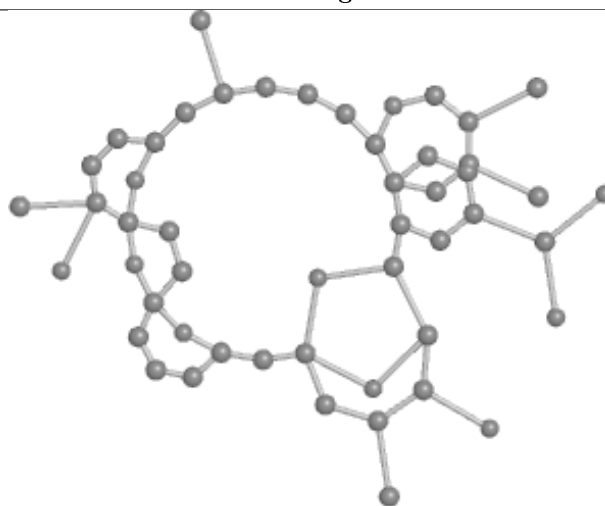
Bond lengths



Bond angles

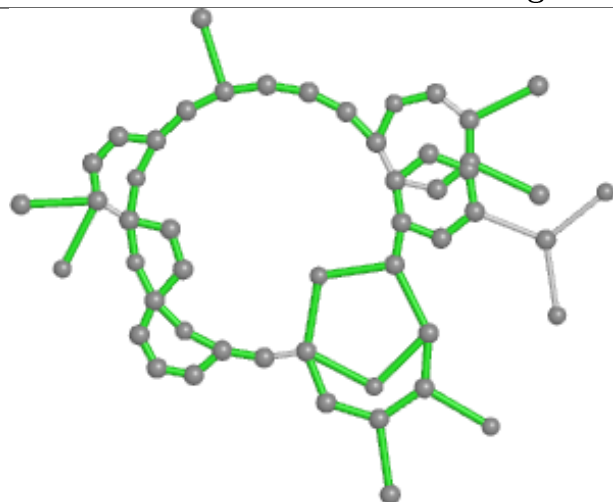


Torsions

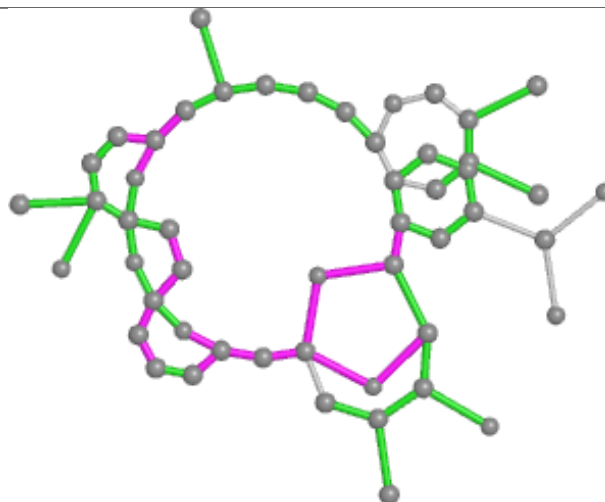


Rings

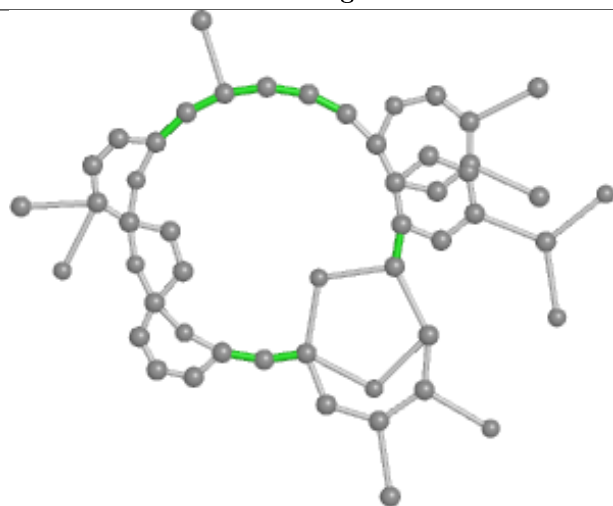
## Ligand 40P I 301



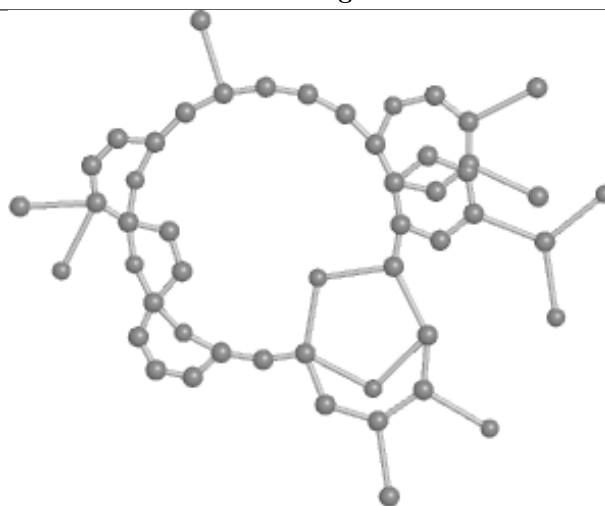
Bond lengths



Bond angles



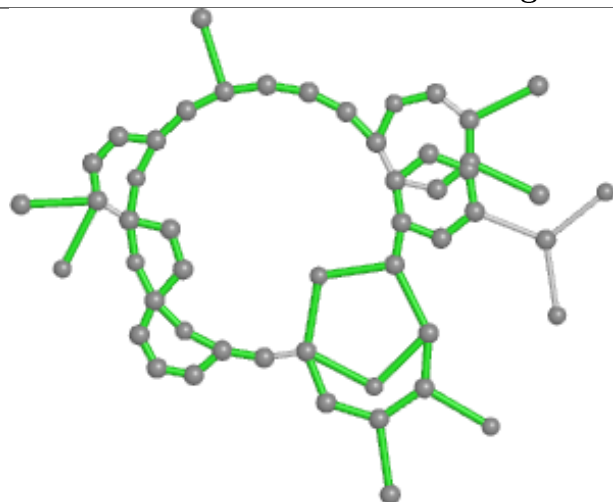
Torsions



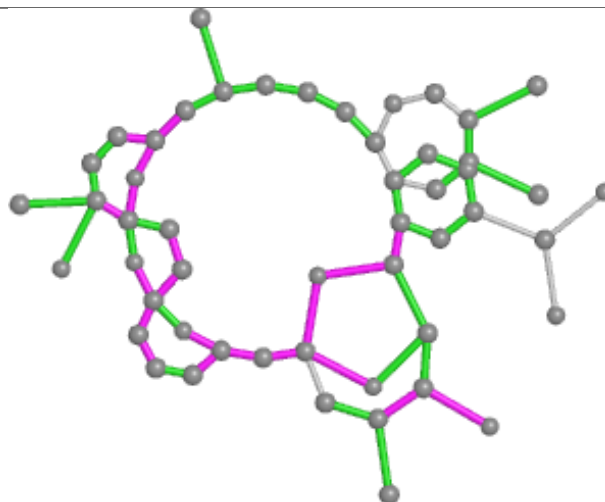
Rings



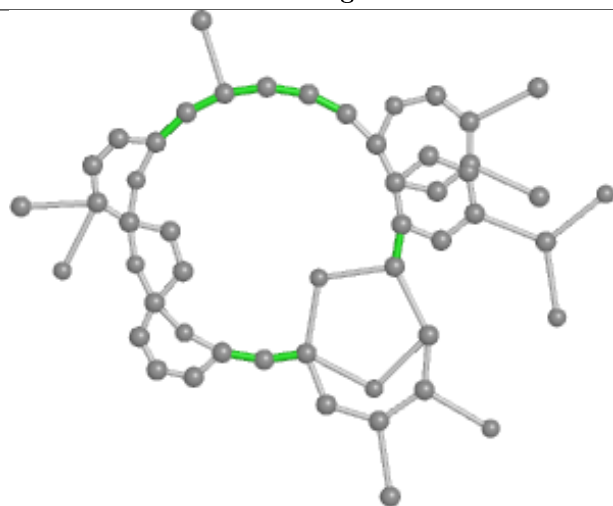
## Ligand 40P H 301



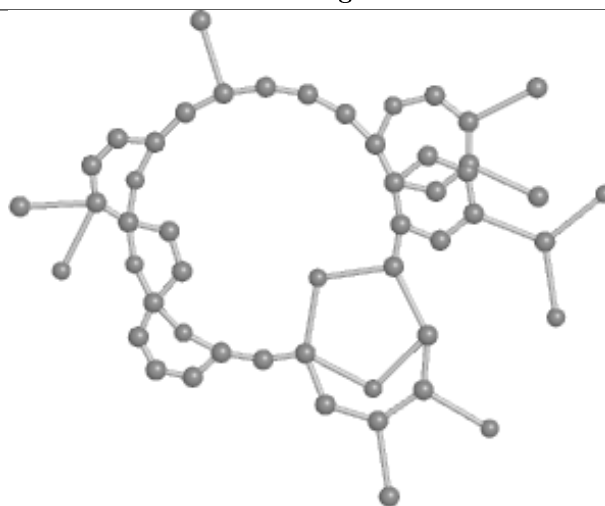
Bond lengths



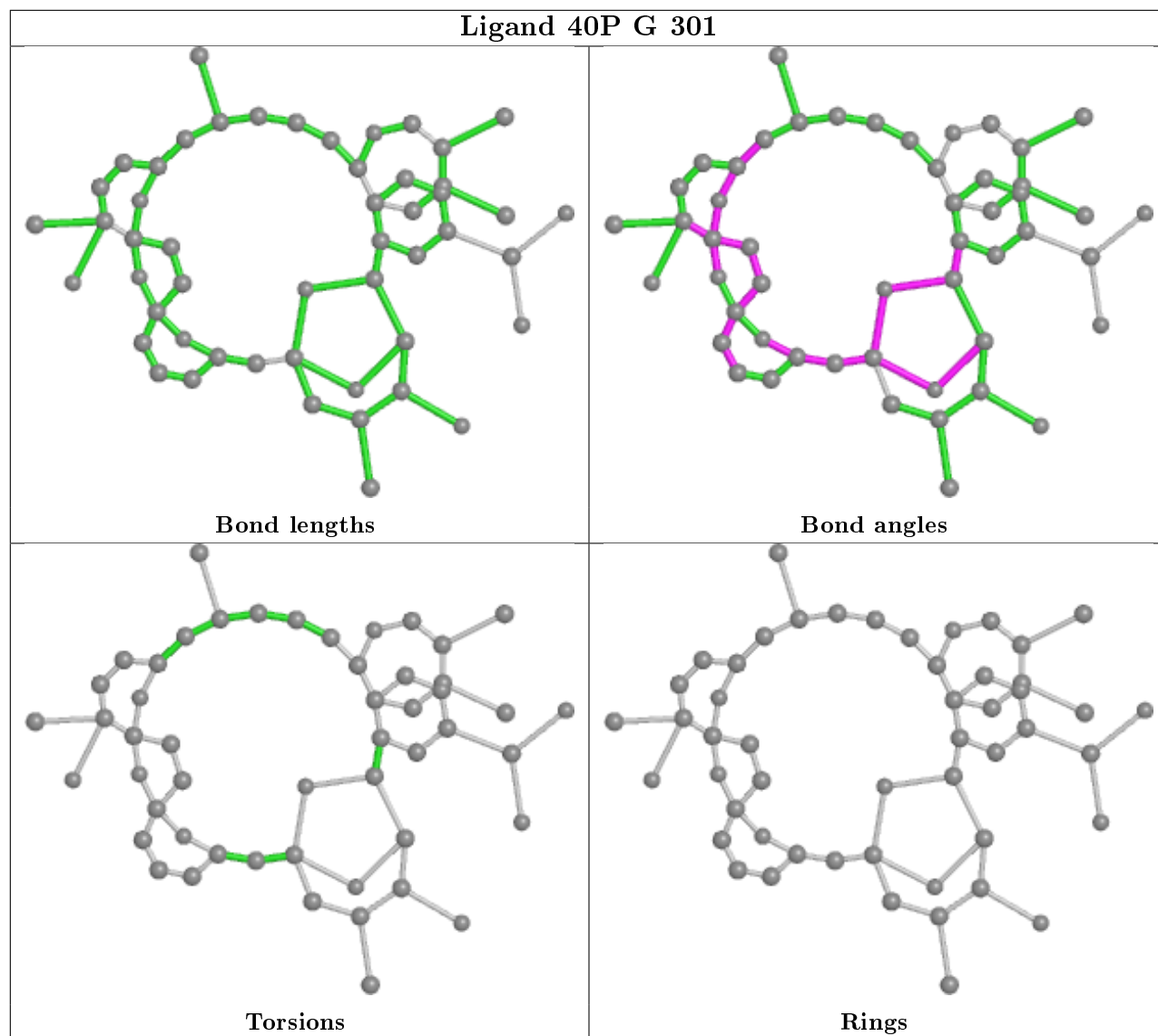
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	216/217 (99%)	0.37	16 (7%) 14 16	13, 24, 54, 78	0
1	B	217/217 (100%)	0.29	14 (6%) 18 21	13, 25, 49, 72	0
1	C	211/217 (97%)	0.25	13 (6%) 20 23	14, 23, 52, 84	0
1	D	211/217 (97%)	0.40	16 (7%) 13 15	15, 26, 61, 84	0
1	E	210/217 (96%)	0.38	13 (6%) 20 23	14, 24, 49, 70	0
1	F	213/217 (98%)	0.34	12 (5%) 24 27	14, 24, 55, 88	0
1	G	210/217 (96%)	0.48	18 (8%) 10 12	14, 26, 57, 82	0
1	H	212/217 (97%)	0.36	15 (7%) 16 17	14, 24, 53, 81	0
1	I	204/217 (94%)	0.30	17 (8%) 11 13	14, 24, 51, 73	0
1	J	211/217 (97%)	0.28	12 (5%) 23 26	13, 25, 50, 79	0
All	All	2115/2170 (97%)	0.34	146 (6%) 16 19	13, 25, 55, 88	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	LEU	9.9
1	J	0	LEU	8.5
1	D	18	PRO	8.4
1	A	18	PRO	8.3
1	E	18	PRO	8.2
1	I	0	LEU	7.8
1	C	18	PRO	7.4
1	F	18	PRO	7.4
1	F	-3	ASP	7.3
1	G	0	LEU	6.8
1	D	0	LEU	6.8
1	I	1	HIS	6.7
1	C	16	ARG	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	-2	ASP	6.3
1	A	-7	TYR	6.2
1	F	-4	ASP	6.2
1	G	-2	ASP	5.9
1	B	18	PRO	5.8
1	G	18	PRO	5.7
1	A	19	MET	5.7
1	J	-1	LYS	5.6
1	F	19	MET	5.5
1	A	16	ARG	5.5
1	E	0	LEU	5.4
1	H	-3	ASP	5.4
1	G	19	MET	5.3
1	D	-1	LYS	5.3
1	F	0	LEU	5.3
1	H	-2	ASP	5.2
1	J	-2	ASP	5.2
1	H	-1	LYS	5.2
1	H	0	LEU	5.1
1	F	16	ARG	5.0
1	D	1	HIS	4.9
1	C	-2	ASP	4.9
1	D	16	ARG	4.8
1	E	-2	ASP	4.8
1	G	16	ARG	4.8
1	B	208	ARG	4.7
1	C	17	SER	4.7
1	A	-6	LYS	4.6
1	C	1	HIS	4.5
1	C	-1	LYS	4.5
1	B	16	ARG	4.3
1	J	208	ARG	4.3
1	A	17	SER	4.2
1	D	208	ARG	4.2
1	J	26	ASP	4.1
1	D	17	SER	4.1
1	B	15	ASN	4.0
1	H	1	HIS	4.0
1	J	18	PRO	3.9
1	C	208	ARG	3.9
1	D	14	PHE	3.9
1	G	-1	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	0	LEU	3.8
1	G	1	HIS	3.8
1	C	19	MET	3.7
1	J	1	HIS	3.6
1	B	14	PHE	3.6
1	I	4	ALA	3.5
1	B	19	MET	3.5
1	G	17	SER	3.5
1	H	14	PHE	3.5
1	F	-2	ASP	3.4
1	A	-3	ASP	3.4
1	F	1	HIS	3.4
1	F	208	ARG	3.4
1	B	17	SER	3.4
1	H	18	PRO	3.4
1	E	1	HIS	3.4
1	I	15	ASN	3.4
1	J	14	PHE	3.4
1	J	19	MET	3.4
1	A	70	ASN	3.3
1	A	74	ASN	3.3
1	A	-5	ASP	3.3
1	D	4	ALA	3.3
1	E	-1	LYS	3.3
1	D	19	MET	3.3
1	G	4	ALA	3.2
1	G	70	ASN	3.2
1	D	70	ASN	3.2
1	H	208	ARG	3.2
1	A	14	PHE	3.2
1	C	14	PHE	3.2
1	H	17	SER	3.1
1	G	14	PHE	3.1
1	I	14	PHE	3.1
1	I	136	GLU	3.1
1	B	1	HIS	3.0
1	G	15	ASN	2.9
1	H	70	ASN	2.9
1	E	17	SER	2.9
1	H	19	MET	2.9
1	H	16	ARG	2.9
1	I	2	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	136	GLU	2.8
1	G	72	TYR	2.8
1	G	136	GLU	2.7
1	B	-4	ASP	2.7
1	E	70	ASN	2.7
1	I	135	GLU	2.6
1	I	20	TYR	2.6
1	I	26	ASP	2.6
1	I	73	GLY	2.6
1	B	-1	LYS	2.5
1	I	72	TYR	2.5
1	E	16	ARG	2.5
1	J	4	ALA	2.4
1	B	-5	ASP	2.4
1	G	74	ASN	2.4
1	E	19	MET	2.4
1	A	208	ARG	2.4
1	A	15	ASN	2.3
1	J	17	SER	2.3
1	D	15	ASN	2.3
1	H	4	ALA	2.3
1	D	72	TYR	2.3
1	E	74	ASN	2.3
1	E	71	GLU	2.2
1	E	11	SER	2.2
1	I	69	PRO	2.2
1	C	207	ARG	2.2
1	A	71	GLU	2.2
1	I	67	TRP	2.2
1	C	70	ASN	2.2
1	G	68	ASP	2.2
1	H	26	ASP	2.2
1	I	71	GLU	2.2
1	H	2	SER	2.2
1	C	7[A]	MET	2.1
1	B	-2	ASP	2.1
1	E	26	ASP	2.1
1	F	70	ASN	2.1
1	B	190	CYS	2.1
1	G	135	GLU	2.1
1	A	-4	ASP	2.1
1	F	15	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	27	ASP	2.1
1	D	71	GLU	2.1
1	J	27	ASP	2.0
1	I	63	ASN	2.0
1	D	27	ASP	2.0
1	A	68	ASP	2.0
1	G	190	CYS	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](#)

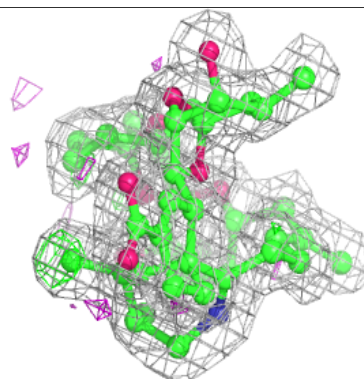
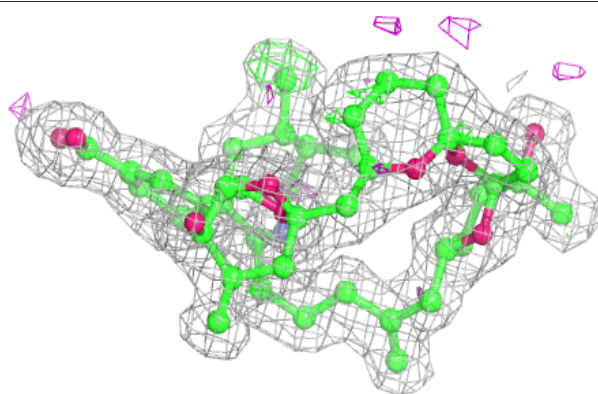
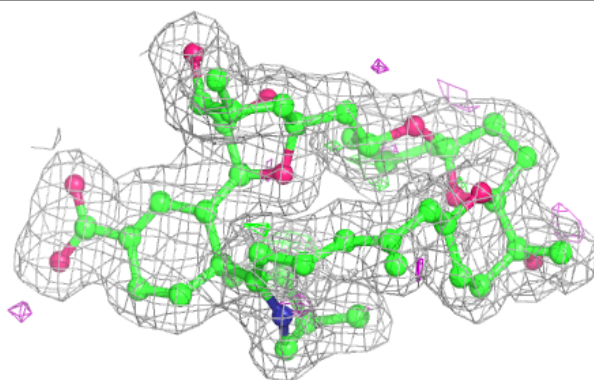
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	E	302	1/1	0.89	0.13	63,63,63,63	0
4	CL	J	302	1/1	0.91	0.10	56,56,56,56	0
2	40P	E	301	51/51	0.94	0.14	21,25,29,31	0
2	40P	G	301	51/51	0.94	0.11	12,21,24,26	0
2	40P	J	301	51/51	0.95	0.10	14,18,22,23	0
2	40P	B	301	51/51	0.95	0.10	15,20,23,24	0
2	40P	A	301	51/51	0.96	0.12	12,17,20,23	0
2	40P	C	301	51/51	0.96	0.10	14,19,22,27	0
2	40P	I	301	51/51	0.96	0.10	12,18,21,24	0
2	40P	H	301	51/51	0.96	0.10	16,20,22,27	0
2	40P	D	301	51/51	0.96	0.10	12,17,22,26	0
2	40P	F	301	51/51	0.97	0.11	12,18,20,23	0
3	CA	D	302	1/1	0.98	0.08	44,44,44,44	0
3	CA	B	302	1/1	0.98	0.09	39,39,39,39	0
3	CA	I	302	1/1	0.99	0.04	36,36,36,36	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 40P E 301:**

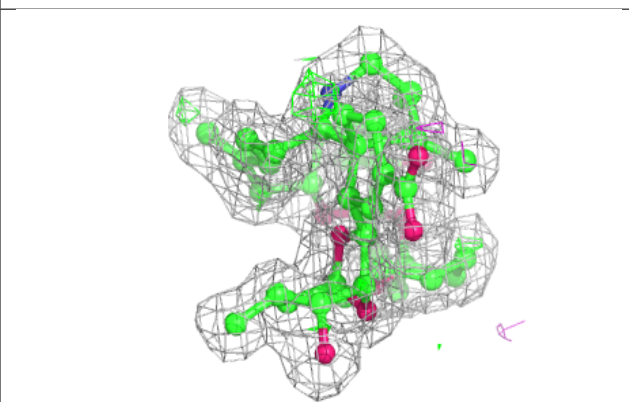
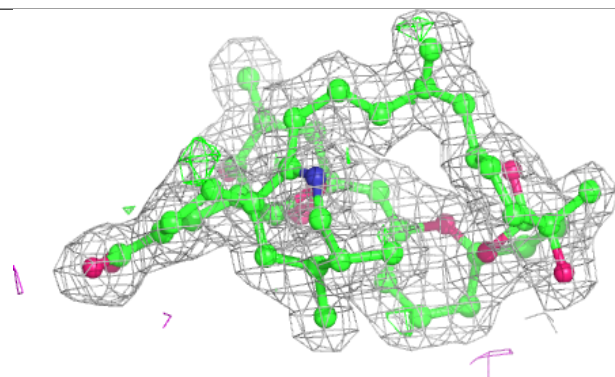
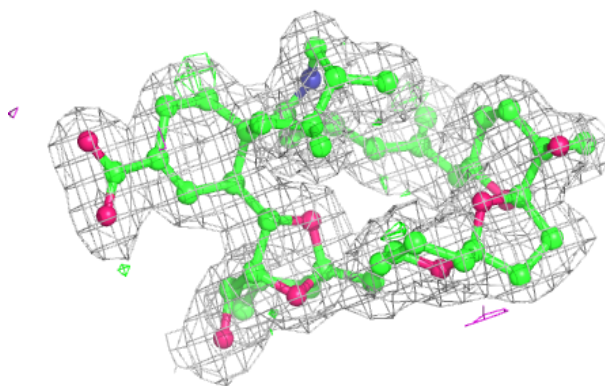
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



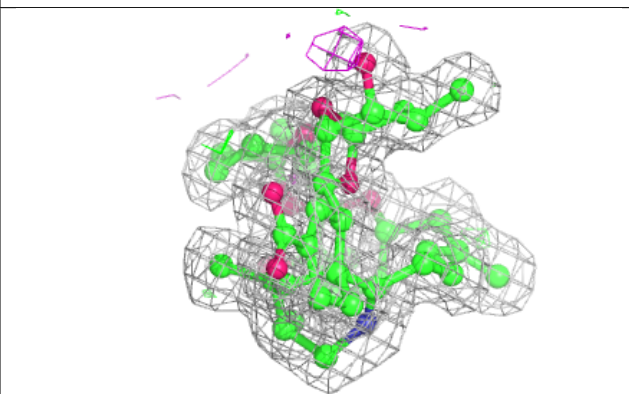
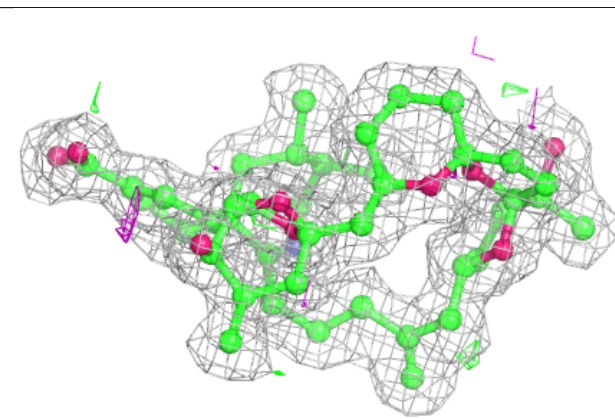
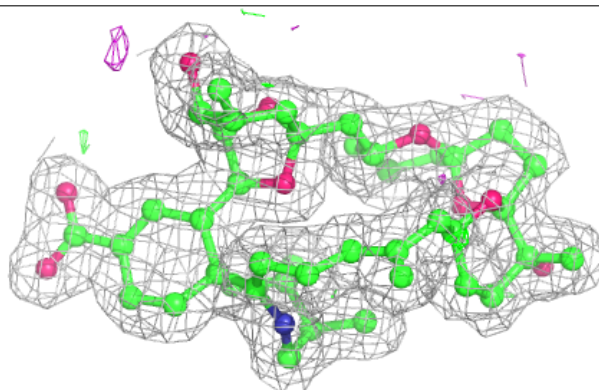


**Electron density around 40P G 301:**

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

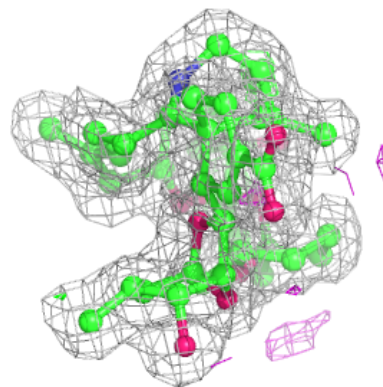
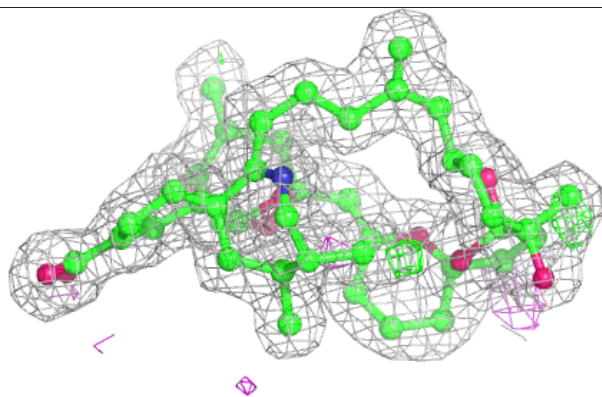
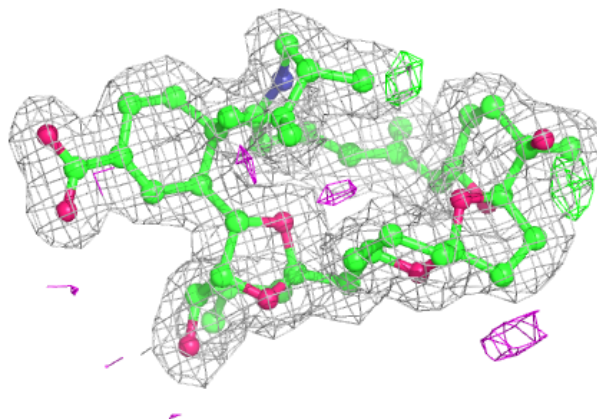
**Electron density around 40P J 301:**

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

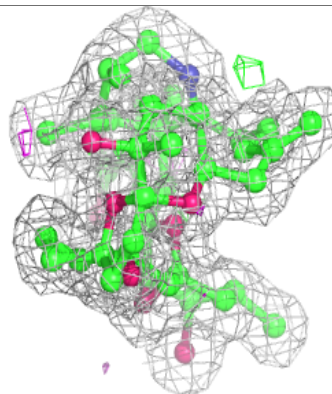
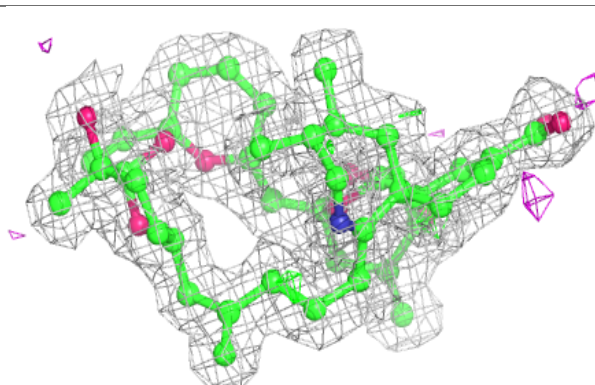
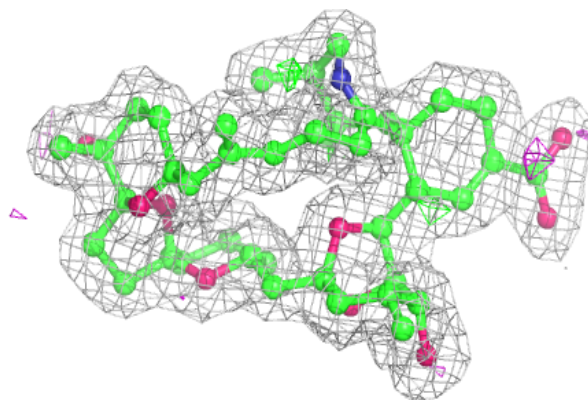


**Electron density around 40P B 301:**

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

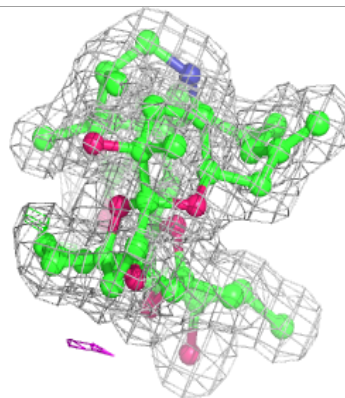
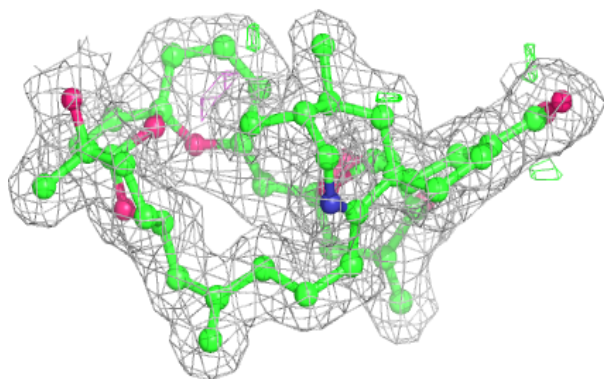
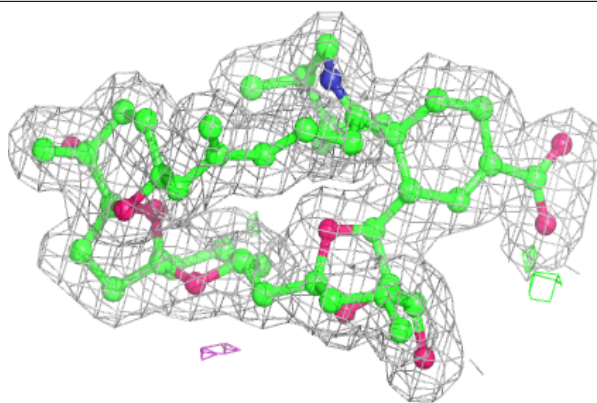
**Electron density around 40P A 301:**

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

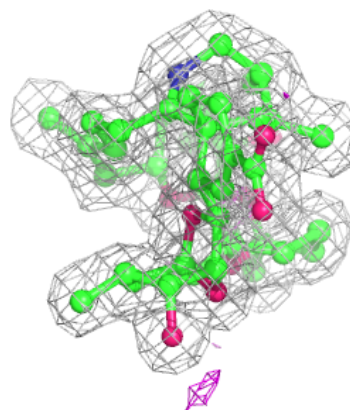
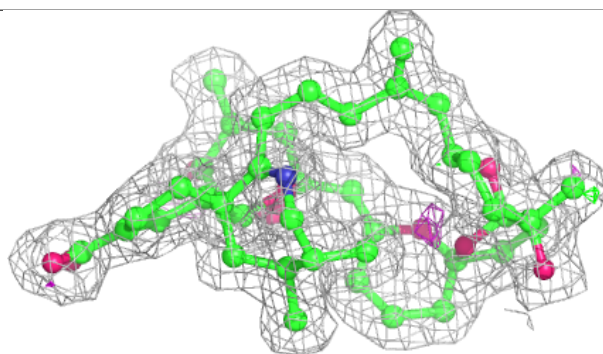
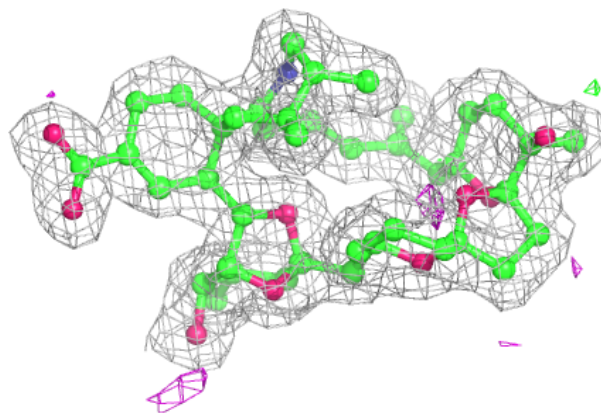


**Electron density around 40P C 301:**

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

**Electron density around 40P I 301:**

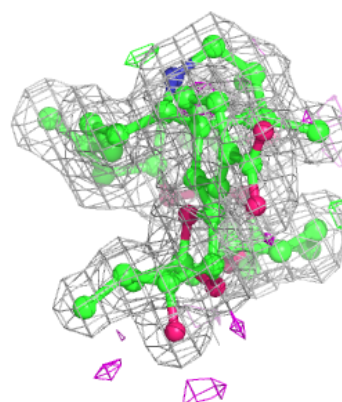
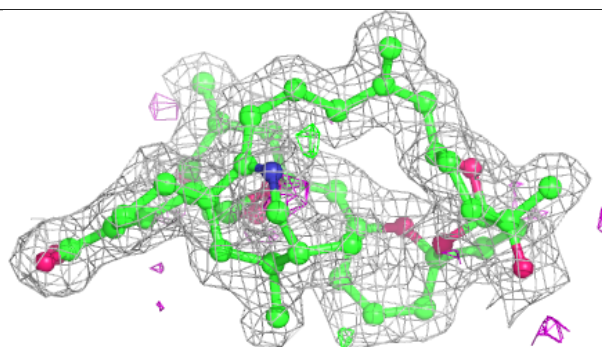
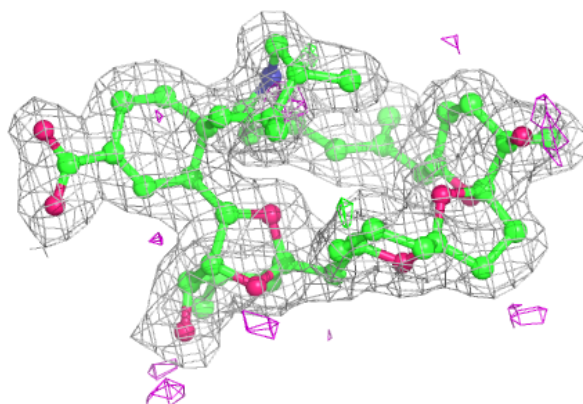
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



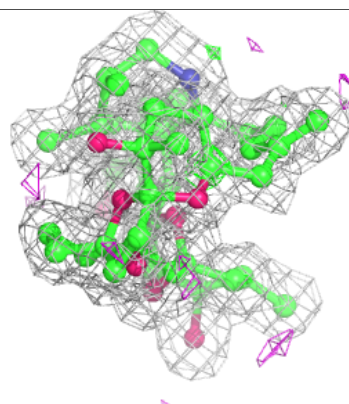
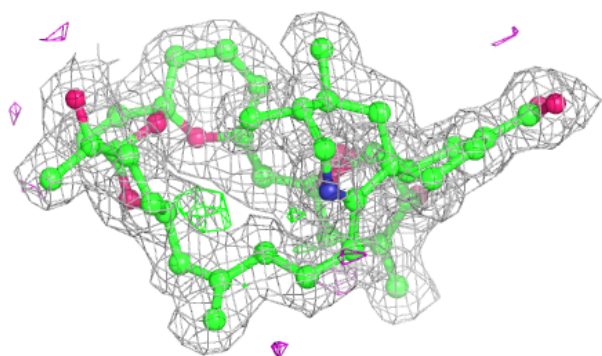
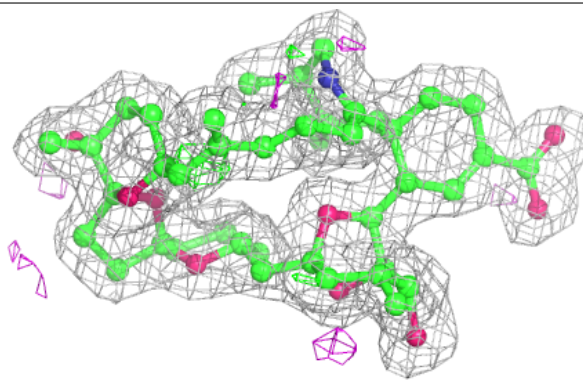


**Electron density around 40P H 301:**

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

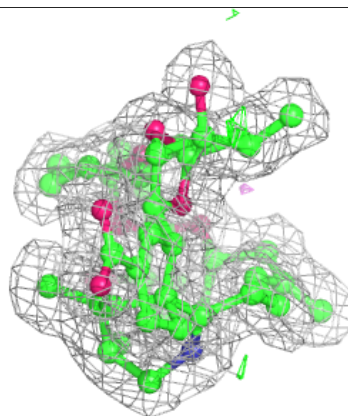
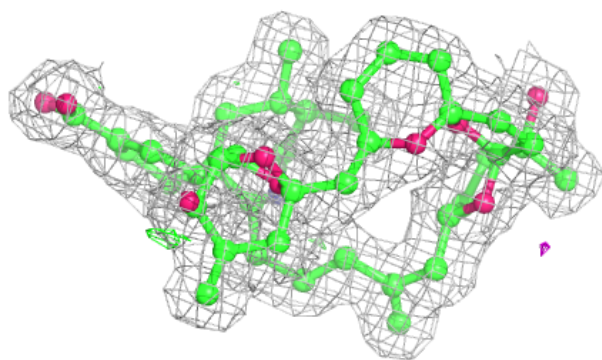
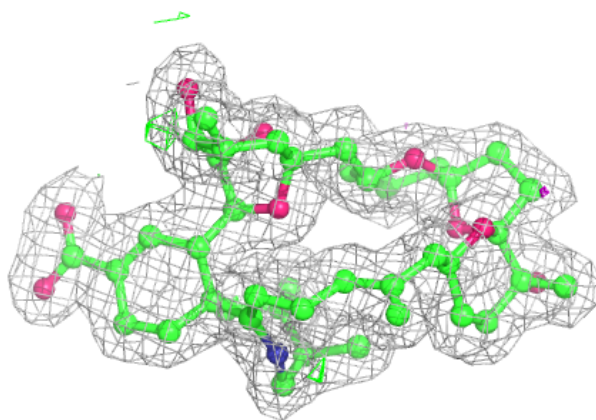
**Electron density around 40P D 301:**

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



**Electron density around 40P F 301:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.