



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 12:08 pm BST

PDB ID : 5MZ2  
Title : Rubisco from *Thalassiosira antarctica*  
Authors : Andersson, I.; Valegard, K.  
Deposited on : 2017-01-30  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

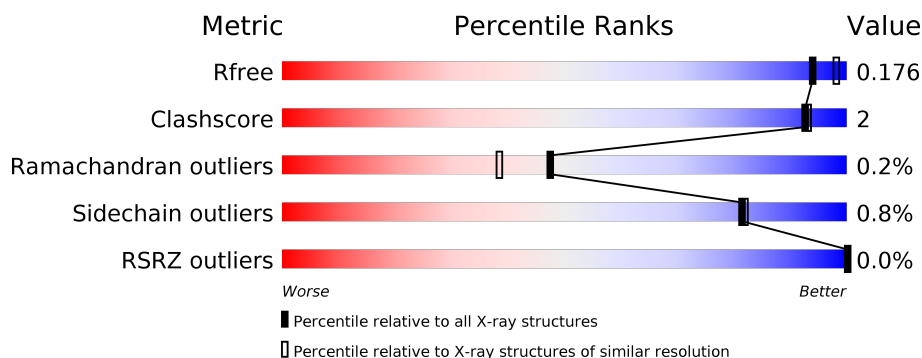
# 1 Overall quality at a glance

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	490	<div> <div>92%</div> <div>6% •</div> </div>
1	B	490	<div> <div>91%</div> <div>7% •</div> </div>
1	C	490	<div> <div>93%</div> <div>5% •</div> </div>
1	D	490	<div> <div>93%</div> <div>5% •</div> </div>
1	E	490	<div> <div>93%</div> <div>5% •</div> </div>
1	F	490	<div> <div>93%</div> <div>6% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	490	 93% 5% •
1	H	490	 93% 5% •
2	I	139	 97% •
2	J	139	 97% •
2	K	139	 99% •
2	L	139	 99% •
2	M	139	 100% •
2	N	139	 99% •
2	O	139	 98% ••
2	P	139	 99% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	HLU	D	174	-	X	-	-
1	HLU	E	174	-	X	-	-
1	HLU	F	174	-	X	-	-
1	HLU	G	174	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42860 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 Rubisco large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3759	2387	646	705	21			
1	C	480	Total	C	N	O	S	0	0	0
			3750	2382	645	702	21			
1	H	481	Total	C	N	O	S	0	0	0
			3759	2387	646	705	21			
1	F	481	Total	C	N	O	S	0	0	0
			3759	2387	646	705	21			
1	D	482	Total	C	N	O	S	0	0	0
			3768	2392	648	707	21			
1	B	480	Total	C	N	O	S	0	0	0
			3750	2382	645	702	21			
1	E	481	Total	C	N	O	S	0	0	0
			3759	2387	646	705	21			
1	G	481	Total	C	N	O	S	0	0	0
			3759	2387	647	704	21			

- Molecule 2 is a protein called Rubisco small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	O	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	L	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	N	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	M	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	P	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			

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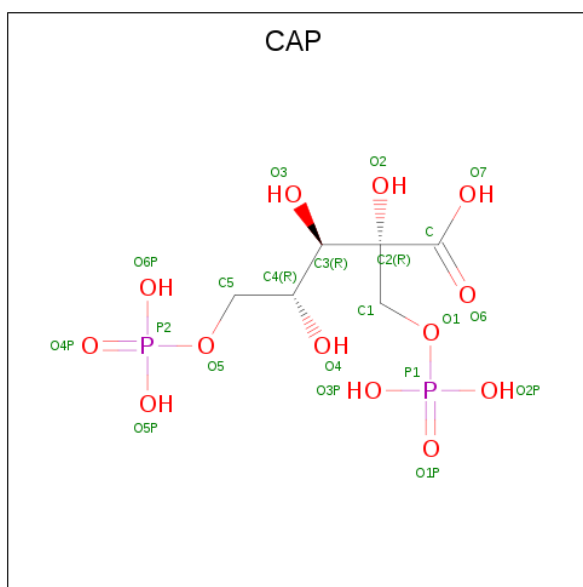
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			
2	K	139	Total	C	N	O	S	0	0	0
			1109	698	189	212	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total 4	C 2	O 2	0	0
5	M	1	Total 4	C 2	O 2	0	0
5	P	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	345	Total 345	O 345	0	0
6	C	349	Total 349	O 349	0	0
6	H	333	Total 333	O 333	0	0
6	F	353	Total 353	O 353	0	0
6	D	368	Total 368	O 368	0	0
6	B	335	Total 335	O 335	0	0
6	E	290	Total 290	O 290	0	0
6	G	313	Total 313	O 313	0	0
6	I	130	Total 130	O 130	0	0
6	O	108	Total 108	O 108	0	0
6	L	121	Total 121	O 121	0	0

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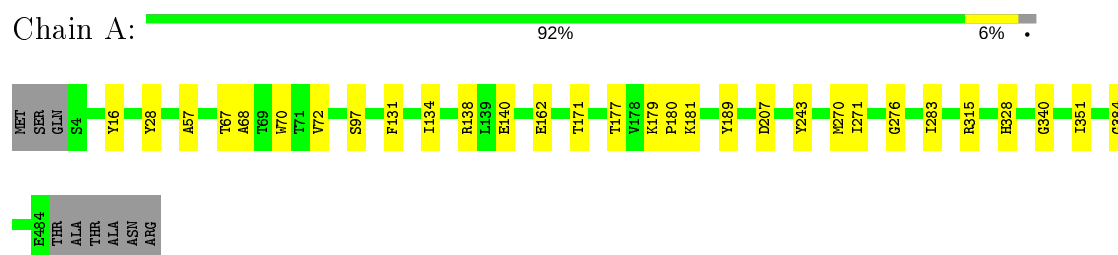
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	123	Total 123	O 123	0	0
6	M	137	Total 137	O 137	0	0
6	P	126	Total 126	O 126	0	0
6	J	131	Total 131	O 131	0	0
6	K	97	Total 97	O 97	0	0

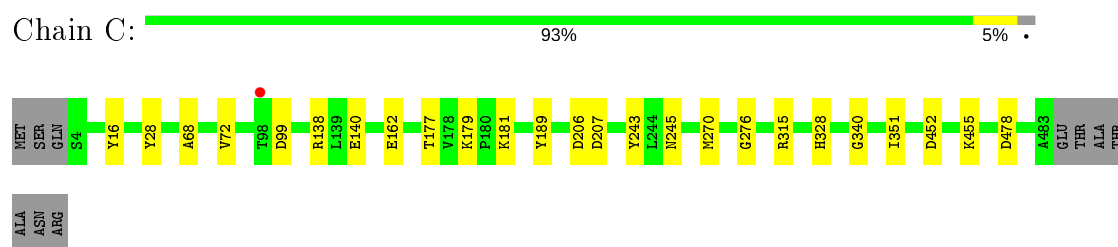
### 3 Residue-property plots [i](#)

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.

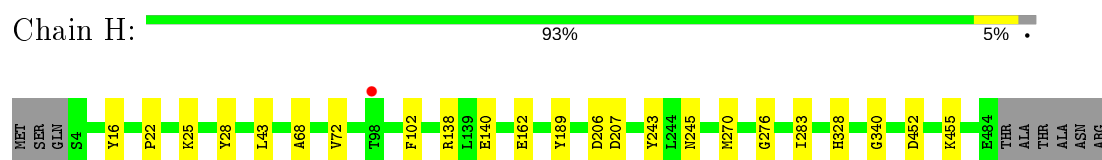
- Molecule 1: Rubisco large subunit



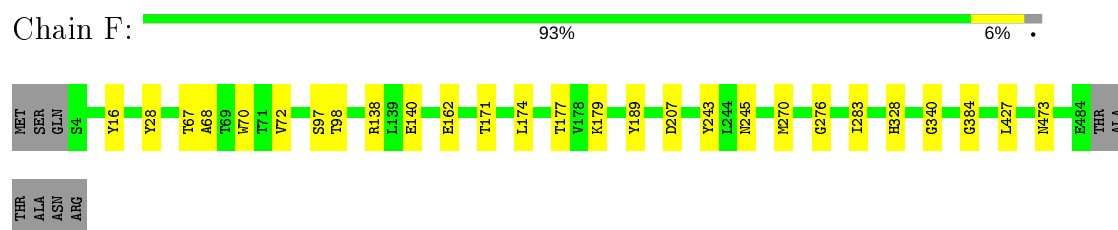
- Molecule 1: Rubisco large subunit




- Molecule 1: Rubisco large subunit



- Molecule 1: Rubisco large subunit




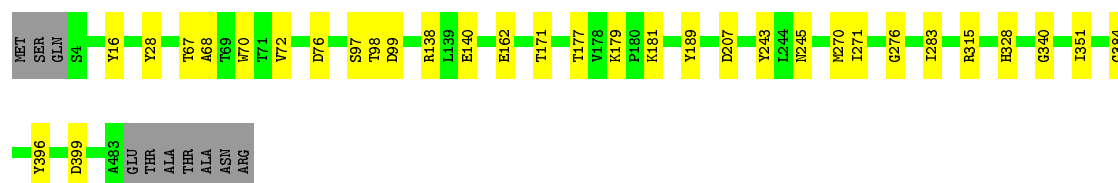
- Molecule 1: Rubisco large subunit

Chain D:  93% 5%



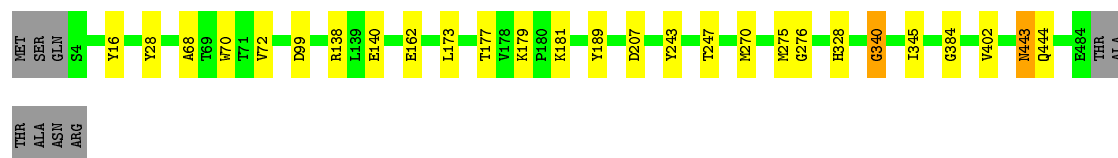
- Molecule 1: Rubisco large subunit

Chain B:  91% 7%



- Molecule 1: Rubisco large subunit

Chain E:  93% 5%



- Molecule 1: Rubisco large subunit

Chain G:  93% 5%



- Molecule 2: Rubisco small subunit

Chain I:  97%



- Molecule 2: Rubisco small subunit

Chain O:  98%



- Molecule 2: Rubisco small subunit

Chain L:  99%



- Molecule 2: Rubisco small subunit

Chain N:  99%



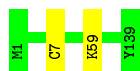
- Molecule 2: Rubisco small subunit

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Rubisco small subunit

Chain P:  99%



- Molecule 2: Rubisco small subunit

Chain J:  97%



- Molecule 2: Rubisco small subunit

Chain K:  99%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.30Å 220.10Å 124.35Å 90.00° 118.39° 90.00°	Depositor
Resolution (Å)	62.09 – 1.90 97.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.09-1.90) 99.8 (97.96-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.143 , 0.175 0.143 , 0.176	Depositor DCC
$R_{free}$ test set	21941 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, HLU, CAP, MG, EDO, HYP, M3L, LYO, KCX

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	0.36	0/3757	0.55	0/5085
1	B	0.36	0/3748	0.56	0/5073
1	C	0.36	0/3748	0.55	0/5073
1	D	0.38	0/3766	0.56	0/5097
1	E	0.37	0/3757	0.56	0/5085
1	F	0.38	0/3757	0.56	0/5085
1	G	0.37	0/3757	0.55	0/5085
1	H	0.36	0/3757	0.55	0/5085
2	I	0.35	0/1137	0.52	0/1540
2	J	0.35	0/1137	0.52	0/1540
2	K	0.34	0/1137	0.52	0/1540
2	L	0.35	0/1137	0.51	0/1540
2	M	0.35	0/1137	0.52	0/1540
2	N	0.34	0/1137	0.51	0/1540
2	O	0.36	0/1137	0.58	2/1540 (0.1%)
2	P	0.36	0/1137	0.52	0/1540
All	All	0.36	0/39143	0.55	2/52988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	119	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	O	119	ARG	NE-CZ-NH1	6.61	123.60	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	A	3759	0	3693	17	0
1	B	3750	0	3687	19	1
1	C	3750	0	3687	16	0
1	D	3768	0	3701	14	0
1	E	3759	0	3693	16	1
1	F	3759	0	3693	15	0
1	G	3759	0	3695	10	0
1	H	3759	0	3693	13	0
2	I	1109	0	1055	5	0
2	J	1109	0	1055	3	0
2	K	1109	0	1055	1	0
2	L	1109	0	1055	1	0
2	M	1109	0	1055	0	0
2	N	1109	0	1055	1	0
2	O	1109	0	1055	2	0
2	P	1109	0	1055	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	M	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	C	21	0	7	0	0
4	D	21	0	8	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	8	0	0
4	H	21	0	7	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	F	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	16	0	24	5	0
5	J	16	0	24	3	0
5	K	4	0	6	0	0
5	L	12	0	18	0	0
5	M	12	0	18	0	0
5	N	4	0	6	0	0
5	O	8	0	12	0	0
5	P	4	0	6	0	0
6	A	345	0	0	0	0
6	B	335	0	0	0	0
6	C	349	0	0	2	0
6	D	368	0	0	2	0
6	E	290	0	0	0	0
6	F	353	0	0	0	0
6	G	313	0	0	0	0
6	H	333	0	0	0	0
6	I	130	0	0	0	0
6	J	131	0	0	0	0
6	K	97	0	0	1	0
6	L	121	0	0	0	0
6	M	137	0	0	0	0
6	N	123	0	0	0	0
6	O	108	0	0	0	0
6	P	126	0	0	0	0
All	All	42860	0	38172	119	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 2.

The worst 5 of 119 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:D:451:ARG:NH1	6:D:1001:HOH:O	2.00	0.94
1:D:468:LYS:NZ	6:D:1001:HOH:O	1.99	0.93
2:I:46:ASN:HD21	5:I:205:EDO:H12	1.44	0.80
1:C:276:GLY:HA3	1:D:276:GLY:HA3	1.65	0.78
1:H:22:PRO:HD2	1:H:25:LYS:HE2	1.64	0.78

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)
1:B:396:TYR:OH	1:E:444:GLN:OE1[1_556]	2.09	0.11

## 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	471/490 (96%)	460 (98%)	10 (2%)	1 (0%)	47	38
1	B	470/490 (96%)	459 (98%)	10 (2%)	1 (0%)	47	38
1	C	470/490 (96%)	459 (98%)	10 (2%)	1 (0%)	47	38
1	D	472/490 (96%)	460 (98%)	11 (2%)	1 (0%)	47	38
1	E	471/490 (96%)	461 (98%)	9 (2%)	1 (0%)	47	38
1	F	471/490 (96%)	462 (98%)	8 (2%)	1 (0%)	47	38
1	G	471/490 (96%)	457 (97%)	13 (3%)	1 (0%)	47	38
1	H	471/490 (96%)	459 (98%)	11 (2%)	1 (0%)	47	38
2	I	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	J	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	K	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	L	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	M	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
2	N	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
2	O	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	P	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
All	All	4863/5032 (97%)	4763 (98%)	92 (2%)	8 (0%)	47	38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLY

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Mol	Chain	Res	Type
1	F	340	GLY
1	B	340	GLY
1	C	340	GLY
1	H	340	GLY

### 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	381/388 (98%)	377 (99%)	4 (1%)	76	76
1	B	380/388 (98%)	376 (99%)	4 (1%)	73	73
1	C	380/388 (98%)	378 (100%)	2 (0%)	88	89
1	D	382/388 (98%)	378 (99%)	4 (1%)	76	76
1	E	381/388 (98%)	378 (99%)	3 (1%)	81	82
1	F	381/388 (98%)	376 (99%)	5 (1%)	69	68
1	G	381/388 (98%)	375 (98%)	6 (2%)	62	60
1	H	381/388 (98%)	379 (100%)	2 (0%)	88	89
2	I	119/119 (100%)	119 (100%)	0	100	100
2	J	119/119 (100%)	119 (100%)	0	100	100
2	K	119/119 (100%)	119 (100%)	0	100	100
2	L	119/119 (100%)	119 (100%)	0	100	100
2	M	119/119 (100%)	119 (100%)	0	100	100
2	N	119/119 (100%)	119 (100%)	0	100	100
2	O	119/119 (100%)	119 (100%)	0	100	100
2	P	119/119 (100%)	118 (99%)	1 (1%)	81	82
All	All	3999/4056 (99%)	3968 (99%)	31 (1%)	81	82

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	169	TYR

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Mol	Chain	Res	Type
1	B	97	SER
1	G	207	ASP
1	D	189	TYR
1	B	189	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	444	GLN
2	I	46	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

64 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	M3L	H	346	1	10,11,12	0.76	0	9,14,16	0.35	0
1	HYP	G	155	1	6,8,9	0.65	0	5,10,12	1.41	0
1	HYP	B	48	1	6,8,9	0.72	0	5,10,12	1.96	2 (40%)
1	HYP	A	155	1	6,8,9	0.61	0	5,10,12	1.26	0
1	HYP	F	48	1	6,8,9	0.68	0	5,10,12	1.62	1 (20%)
1	CSO	A	109	1	3,6,7	0.71	0	0,6,8	0.00	-
1	CSO	D	109	1	3,6,7	0.75	0	0,6,8	0.00	-
1	KCX	A	205	1,3	7,11,12	1.24	1 (14%)	4,12,14	0.48	0
1	HYP	A	48	1	6,8,9	0.75	0	5,10,12	2.09	2 (40%)
1	HYP	C	48	1	6,8,9	0.67	0	5,10,12	2.08	2 (40%)
1	LYO	B	150	1	7,9,10	0.37	0	6,10,12	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	M3L	F	346	1	10,11,12	0.77	0	9,14,16	0.43	0
1	LYO	F	150	1	7,9,10	0.45	0	6,10,12	0.70	0
1	LYO	C	198	1	7,9,10	0.37	0	6,10,12	0.86	0
1	LYO	D	198	1	7,9,10	0.35	0	6,10,12	0.79	0
1	HYP	D	48	1	6,8,9	0.64	0	5,10,12	2.18	2 (40%)
1	LYO	D	150	1	7,9,10	0.47	0	6,10,12	0.75	0
1	HYP	E	155	1	6,8,9	0.58	0	5,10,12	1.26	0
1	CSO	C	109	1	3,6,7	0.78	0	0,6,8	0.00	-
1	HLU	A	174	1	7,8,9	0.72	0	7,10,12	2.01	3 (42%)
1	HYP	F	155	1	6,8,9	0.57	0	5,10,12	1.26	0
1	KCX	C	205	1,3	7,11,12	1.00	1 (14%)	4,12,14	0.21	0
1	HYP	G	48	1	6,8,9	0.65	0	5,10,12	1.96	2 (40%)
1	LYO	H	150	1	7,9,10	0.48	0	6,10,12	0.73	0
1	LYO	E	198	1	7,9,10	0.43	0	6,10,12	0.84	0
1	M3L	A	346	1	10,11,12	0.76	0	9,14,16	0.31	0
1	LYO	G	198	1	7,9,10	0.33	0	6,10,12	0.95	0
1	LYO	E	150	1	7,9,10	0.46	0	6,10,12	0.79	0
1	LYO	B	198	1	7,9,10	0.45	0	6,10,12	0.93	0
1	KCX	G	205	1,3	7,11,12	1.01	1 (14%)	4,12,14	0.61	0
1	HLU	F	174	1	7,8,9	0.73	0	7,10,12	2.16	4 (57%)
1	M3L	G	346	1	10,11,12	0.75	0	9,14,16	0.39	0
1	HYP	H	48	1	6,8,9	0.68	0	5,10,12	2.05	2 (40%)
1	HLU	C	174	1	7,8,9	0.77	0	7,10,12	1.87	3 (42%)
1	LYO	H	198	1	7,9,10	0.37	0	6,10,12	0.72	0
1	HLU	G	174	1	7,8,9	0.78	0	7,10,12	2.30	4 (57%)
1	HLU	B	174	1	7,8,9	0.79	0	7,10,12	2.06	3 (42%)
1	HLU	E	174	1	7,8,9	0.72	0	7,10,12	2.30	4 (57%)
1	CSO	H	109	1	3,6,7	0.79	0	0,6,8	0.00	-
1	CSO	F	109	1	3,6,7	0.63	0	0,6,8	0.00	-
1	KCX	H	205	1,3	7,11,12	0.96	1 (14%)	4,12,14	0.32	0
1	HYP	H	155	1	6,8,9	0.70	0	5,10,12	1.52	1 (20%)
1	HYP	B	155	1	6,8,9	0.61	0	5,10,12	1.07	0
1	LYO	A	150	1	7,9,10	0.39	0	6,10,12	0.72	0
1	LYO	C	150	1	7,9,10	0.43	0	6,10,12	1.00	0
1	HYP	C	155	1	6,8,9	0.77	0	5,10,12	1.48	1 (20%)
1	LYO	A	198	1	7,9,10	0.45	0	6,10,12	0.82	0
1	M3L	D	346	1	10,11,12	0.79	0	9,14,16	0.37	0
1	M3L	C	346	1	10,11,12	0.78	0	9,14,16	0.35	0
1	KCX	B	205	1,3	7,11,12	1.13	1 (14%)	4,12,14	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	F	205	1,3	7,11,12	0.96	0	4,12,14	0.33	0
1	KCX	D	205	1,3	7,11,12	1.10	1 (14%)	4,12,14	0.30	0
1	HLU	D	174	1	7,8,9	0.79	0	7,10,12	2.26	4 (57%)
1	CSO	G	109	1	3,6,7	0.82	0	0,6,8	0.00	-
1	CSO	B	109	1	3,6,7	0.75	0	0,6,8	0.00	-
1	CSO	E	109	1	3,6,7	0.71	0	0,6,8	0.00	-
1	HLU	H	174	1	7,8,9	0.78	0	7,10,12	1.90	3 (42%)
1	KCX	E	205	1,3	7,11,12	1.00	0	4,12,14	0.46	0
1	HYP	E	48	1	6,8,9	0.71	0	5,10,12	1.76	2 (40%)
1	HYP	D	155	1	6,8,9	0.62	0	5,10,12	1.44	0
1	M3L	B	346	1	10,11,12	0.77	0	9,14,16	0.31	0
1	LYO	F	198	1	7,9,10	0.44	0	6,10,12	0.80	0
1	M3L	E	346	1	10,11,12	0.76	0	9,14,16	0.42	0
1	LYO	G	150	1	7,9,10	0.44	0	6,10,12	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	H	346	1	-	1/9/10/12	-
1	HYP	G	155	1	-	0/0/11/13	0/1/1/1
1	HYP	B	48	1	-	0/0/11/13	0/1/1/1
1	HYP	A	155	1	-	0/0/11/13	0/1/1/1
1	HYP	F	48	1	-	0/0/11/13	0/1/1/1
1	CSO	A	109	1	-	0/1/5/7	-
1	CSO	D	109	1	-	0/1/5/7	-
1	KCX	A	205	1,3	-	0/7/10/12	-
1	HYP	A	48	1	-	0/0/11/13	0/1/1/1
1	HYP	C	48	1	-	0/0/11/13	0/1/1/1
1	LYO	B	150	1	-	1/8/9/11	-
1	M3L	F	346	1	-	1/9/10/12	-
1	LYO	F	150	1	-	1/8/9/11	-
1	LYO	C	198	1	-	1/8/9/11	-
1	LYO	D	198	1	-	1/8/9/11	-
1	HYP	D	48	1	-	0/0/11/13	0/1/1/1
1	LYO	D	150	1	-	1/8/9/11	-
1	HYP	E	155	1	-	0/0/11/13	0/1/1/1
1	CSO	C	109	1	-	0/1/5/7	-
1	HLU	A	174	1	-	8/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	F	155	1	-	0/0/11/13	0/1/1/1
1	KCX	C	205	1,3	-	0/7/10/12	-
1	HYP	G	48	1	-	0/0/11/13	0/1/1/1
1	LYO	H	150	1	-	1/8/9/11	-
1	LYO	E	198	1	-	1/8/9/11	-
1	M3L	A	346	1	-	1/9/10/12	-
1	LYO	G	198	1	-	1/8/9/11	-
1	LYO	E	150	1	-	1/8/9/11	-
1	LYO	B	198	1	-	1/8/9/11	-
1	KCX	G	205	1,3	-	0/7/10/12	-
1	HLU	F	174	1	-	8/9/10/12	-
1	M3L	G	346	1	-	1/9/10/12	-
1	HYP	H	48	1	-	0/0/11/13	0/1/1/1
1	HLU	C	174	1	-	8/9/10/12	-
1	LYO	H	198	1	-	1/8/9/11	-
1	HLU	G	174	1	-	8/9/10/12	-
1	HLU	B	174	1	-	8/9/10/12	-
1	HLU	E	174	1	-	8/9/10/12	-
1	CSO	H	109	1	-	0/1/5/7	-
1	CSO	F	109	1	-	0/1/5/7	-
1	KCX	H	205	1,3	-	0/7/10/12	-
1	HYP	H	155	1	-	0/0/11/13	0/1/1/1
1	HYP	B	155	1	-	0/0/11/13	0/1/1/1
1	LYO	A	150	1	-	1/8/9/11	-
1	LYO	C	150	1	-	0/8/9/11	-
1	HYP	C	155	1	-	0/0/11/13	0/1/1/1
1	LYO	A	198	1	-	0/8/9/11	-
1	M3L	D	346	1	-	1/9/10/12	-
1	M3L	C	346	1	-	1/9/10/12	-
1	KCX	B	205	1,3	-	0/7/10/12	-
1	KCX	F	205	1,3	-	0/7/10/12	-
1	KCX	D	205	1,3	-	0/7/10/12	-
1	HLU	D	174	1	-	8/9/10/12	-
1	CSO	G	109	1	-	0/1/5/7	-
1	CSO	B	109	1	-	0/1/5/7	-
1	CSO	E	109	1	-	0/1/5/7	-
1	HLU	H	174	1	-	8/9/10/12	-
1	KCX	E	205	1,3	-	0/7/10/12	-
1	HYP	E	48	1	-	0/0/11/13	0/1/1/1
1	HYP	D	155	1	-	0/0/11/13	0/1/1/1
1	M3L	B	346	1	-	1/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYO	F	198	1	-	0/8/9/11	-
1	M3L	E	346	1	-	1/9/10/12	-
1	LYO	G	150	1	-	1/8/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	KCX	CE-NZ	2.84	1.51	1.45
1	B	205	KCX	CE-NZ	2.51	1.51	1.45
1	D	205	KCX	CE-NZ	2.45	1.51	1.45
1	C	205	KCX	CE-NZ	2.18	1.50	1.45
1	G	205	KCX	CE-NZ	2.16	1.50	1.45

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	HLU	OH-CB-CG	3.77	117.77	109.89
1	D	174	HLU	OH-CB-CG	3.69	117.59	109.89
1	G	174	HLU	OH-CB-CG	3.67	117.56	109.89
1	F	174	HLU	OH-CB-CG	3.51	117.22	109.89
1	A	174	HLU	OH-CB-CG	3.46	117.12	109.89

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	174	HLU	N-CA-CB-CG
1	H	174	HLU	N-CA-CB-OH
1	H	174	HLU	C-CA-CB-CG
1	H	174	HLU	C-CA-CB-OH
1	H	174	HLU	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	198	LYO	1	0
1	F	174	HLU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	$\# Z  > 2$
4	CAP	B	902	3	15,20,20	0.62	0	20,31,31	0.97	0
5	EDO	J	201	-	3,3,3	0.37	0	2,2,2	0.51	0
4	CAP	G	902	3	15,20,20	0.59	0	20,31,31	0.92	0
5	EDO	M	204	-	3,3,3	0.40	0	2,2,2	0.50	0
5	EDO	L	203	-	3,3,3	0.49	0	2,2,2	0.21	0
5	EDO	F	903	-	3,3,3	0.52	0	2,2,2	0.11	0
5	EDO	J	203	-	3,3,3	0.49	0	2,2,2	0.22	0
4	CAP	D	902	3	15,20,20	0.62	0	20,31,31	0.92	0
4	CAP	F	902	3	15,20,20	0.59	0	20,31,31	0.93	0
5	EDO	N	201	-	3,3,3	0.45	0	2,2,2	0.20	0
5	EDO	L	201	-	3,3,3	0.40	0	2,2,2	0.61	0
4	CAP	E	902	3	15,20,20	0.60	0	20,31,31	0.89	0
5	EDO	I	204	-	3,3,3	0.49	0	2,2,2	0.18	0
4	CAP	A	902	3	15,20,20	0.68	0	20,31,31	0.89	0
5	EDO	O	201	-	3,3,3	0.48	0	2,2,2	0.22	0
5	EDO	A	903	-	3,3,3	0.45	0	2,2,2	0.15	0
5	EDO	I	202	-	3,3,3	0.42	0	2,2,2	0.46	0
5	EDO	I	203	-	3,3,3	0.41	0	2,2,2	0.16	0
5	EDO	J	204	-	3,3,3	0.42	0	2,2,2	0.21	0
5	EDO	K	201	-	3,3,3	0.38	0	2,2,2	0.40	0
5	EDO	J	202	-	3,3,3	0.40	0	2,2,2	0.26	0
5	EDO	O	202	-	3,3,3	0.44	0	2,2,2	0.23	0
5	EDO	L	202	-	3,3,3	0.42	0	2,2,2	0.28	0
5	EDO	P	201	-	3,3,3	0.51	0	2,2,2	0.13	0
5	EDO	M	203	-	3,3,3	0.48	0	2,2,2	0.31	0
4	CAP	C	902	3	15,20,20	0.72	0	20,31,31	0.90	0
5	EDO	I	205	-	3,3,3	0.39	0	2,2,2	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAP	H	902	3	15,20,20	0.70	0	20,31,31	0.93	0
5	EDO	B	903	-	3,3,3	0.53	0	2,2,2	0.19	0
5	EDO	M	202	-	3,3,3	0.49	0	2,2,2	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	B	902	3	-	3/23/29/29	-
5	EDO	J	201	-	-	0/1/1/1	-
4	CAP	G	902	3	-	3/23/29/29	-
5	EDO	M	204	-	-	0/1/1/1	-
5	EDO	L	203	-	-	0/1/1/1	-
5	EDO	F	903	-	-	0/1/1/1	-
5	EDO	J	203	-	-	0/1/1/1	-
4	CAP	D	902	3	-	2/23/29/29	-
4	CAP	F	902	3	-	3/23/29/29	-
5	EDO	N	201	-	-	0/1/1/1	-
5	EDO	L	201	-	-	0/1/1/1	-
4	CAP	E	902	3	-	3/23/29/29	-
5	EDO	I	204	-	-	0/1/1/1	-
4	CAP	A	902	3	-	3/23/29/29	-
5	EDO	O	201	-	-	0/1/1/1	-
5	EDO	A	903	-	-	0/1/1/1	-
5	EDO	I	202	-	-	0/1/1/1	-
5	EDO	I	203	-	-	0/1/1/1	-
5	EDO	J	204	-	-	0/1/1/1	-
5	EDO	K	201	-	-	0/1/1/1	-
5	EDO	J	202	-	-	1/1/1/1	-
5	EDO	O	202	-	-	0/1/1/1	-
5	EDO	L	202	-	-	0/1/1/1	-
5	EDO	P	201	-	-	0/1/1/1	-
5	EDO	M	203	-	-	0/1/1/1	-
4	CAP	C	902	3	-	3/23/29/29	-
5	EDO	I	205	-	-	0/1/1/1	-
4	CAP	H	902	3	-	3/23/29/29	-
5	EDO	B	903	-	-	0/1/1/1	-
5	EDO	M	202	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

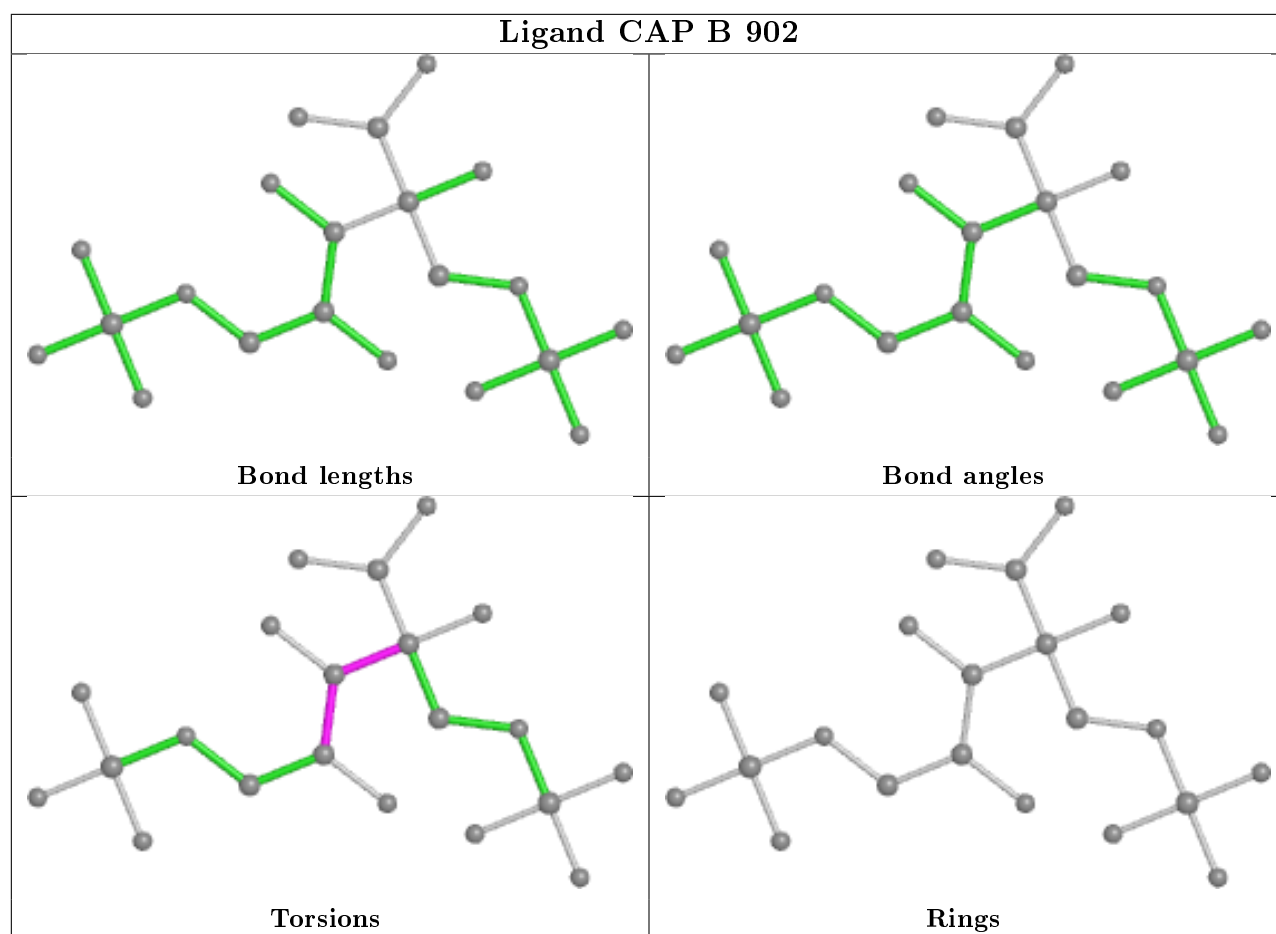
Mol	Chain	Res	Type	Atoms
4	B	902	CAP	C2-C3-C4-O4
4	B	902	CAP	O3-C3-C4-O4
4	G	902	CAP	O3-C3-C4-O4
4	D	902	CAP	O3-C3-C4-O4
4	F	902	CAP	O3-C3-C4-O4

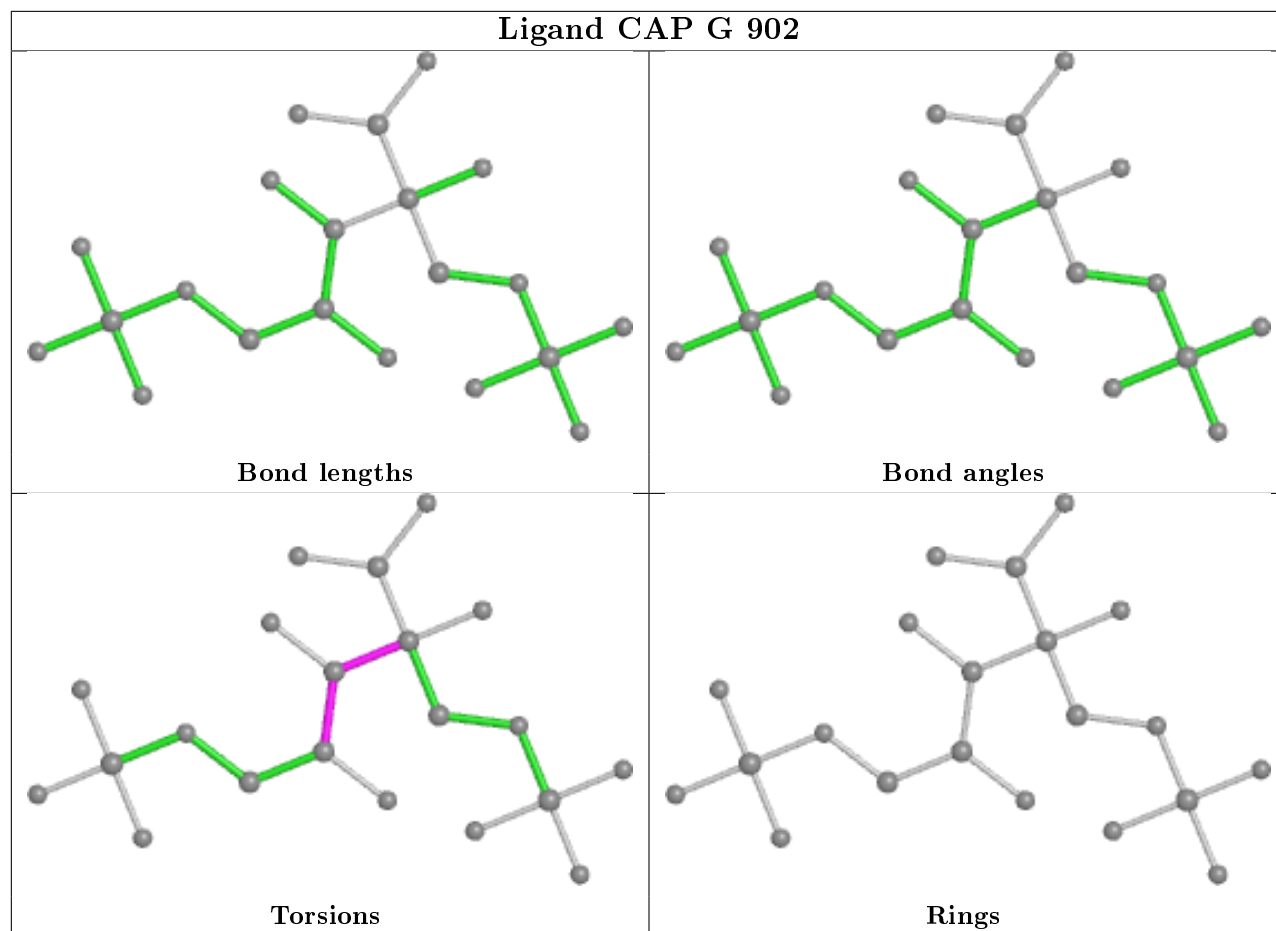
There are no ring outliers.

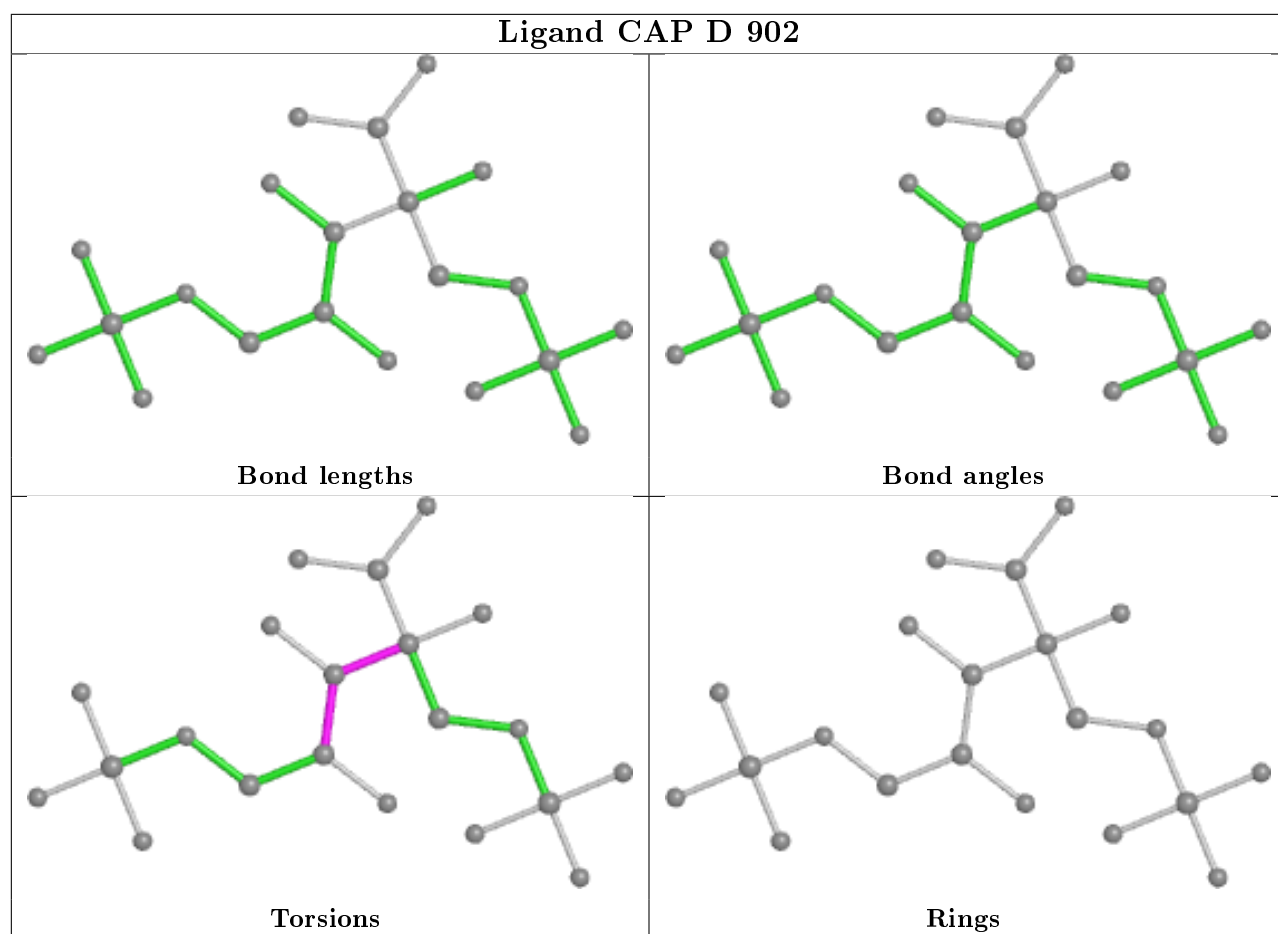
3 monomers are involved in 7 short contacts:

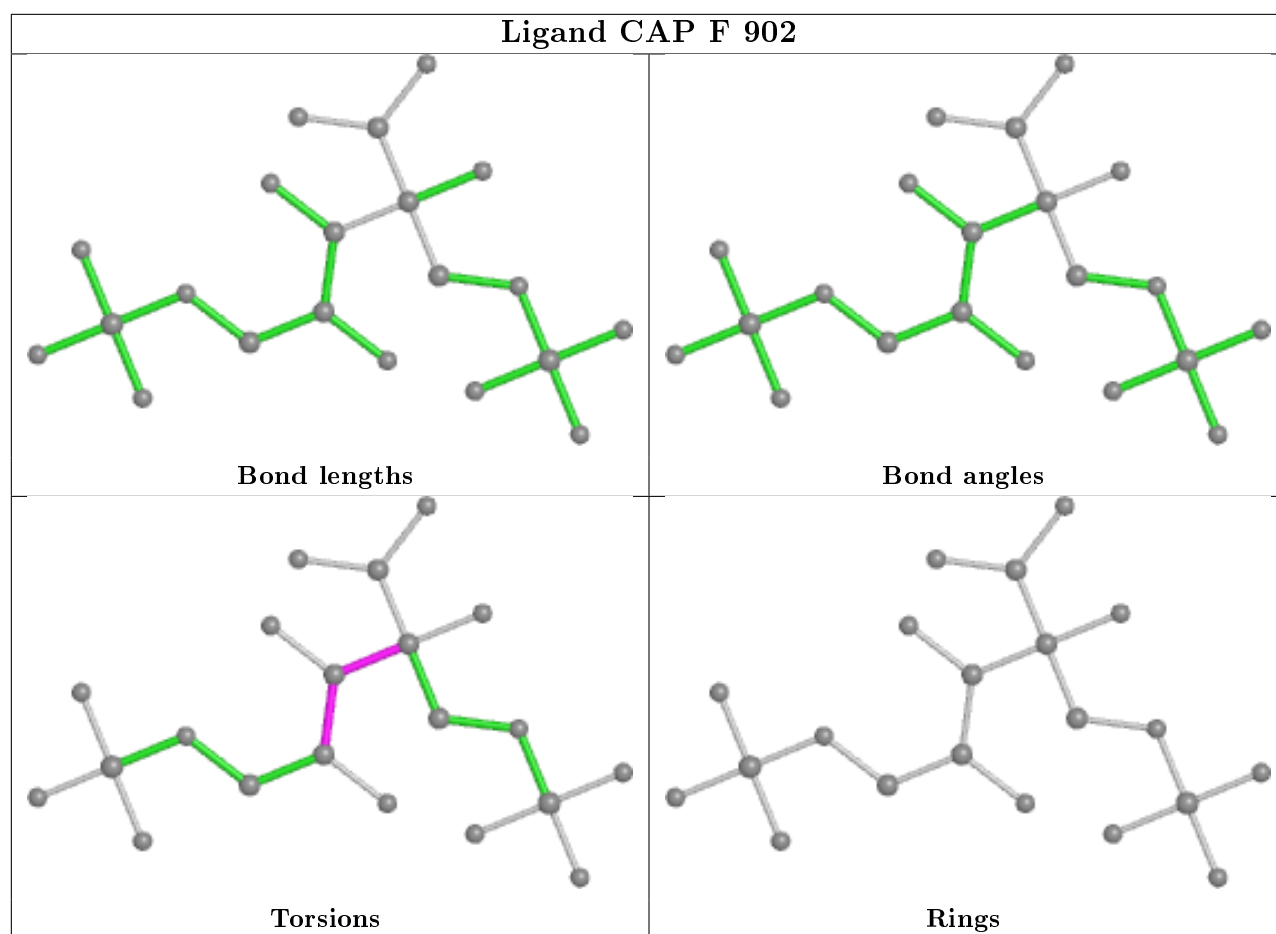
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	203	EDO	3	0
5	J	202	EDO	3	0
5	I	205	EDO	2	0

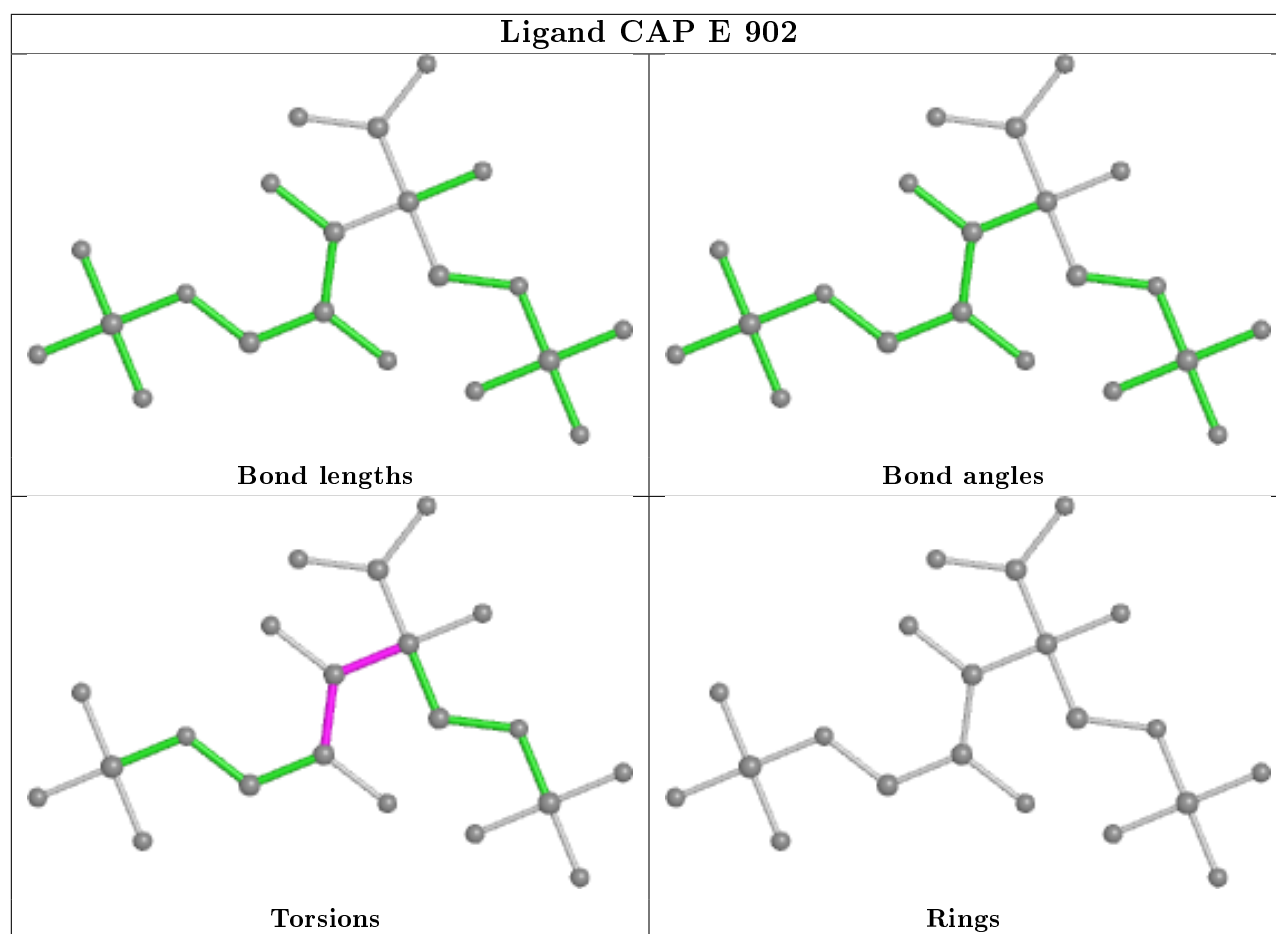
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

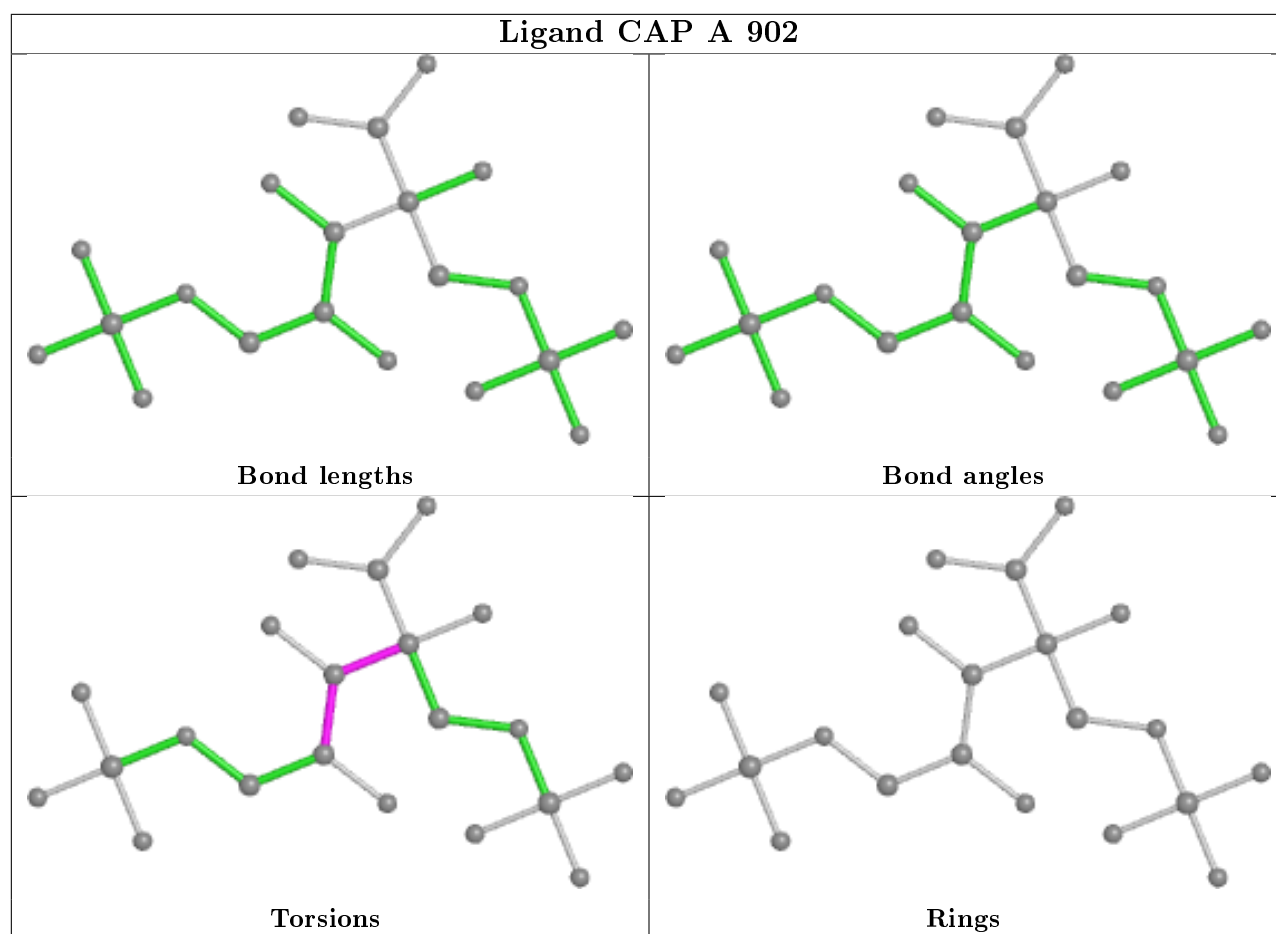




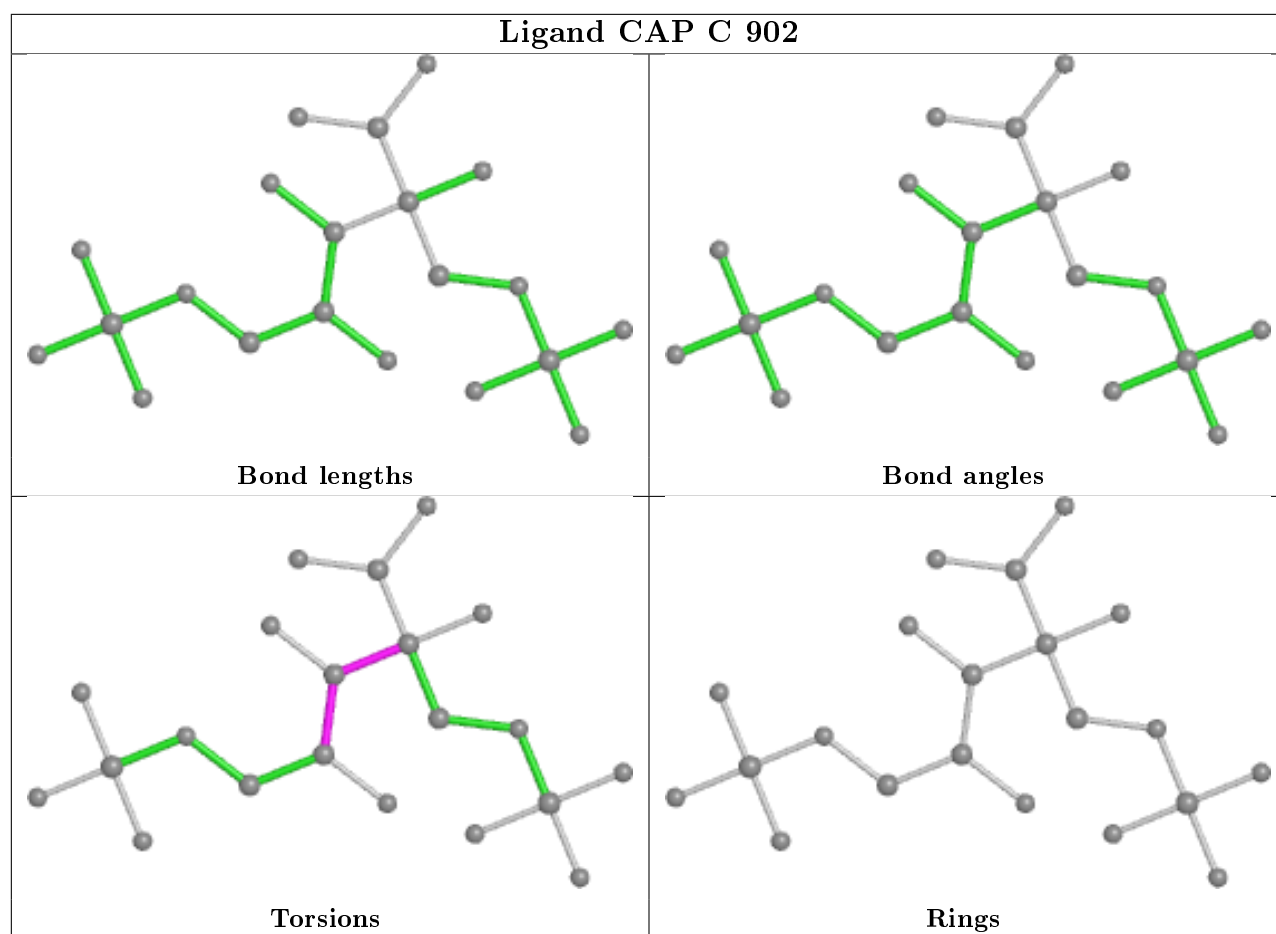


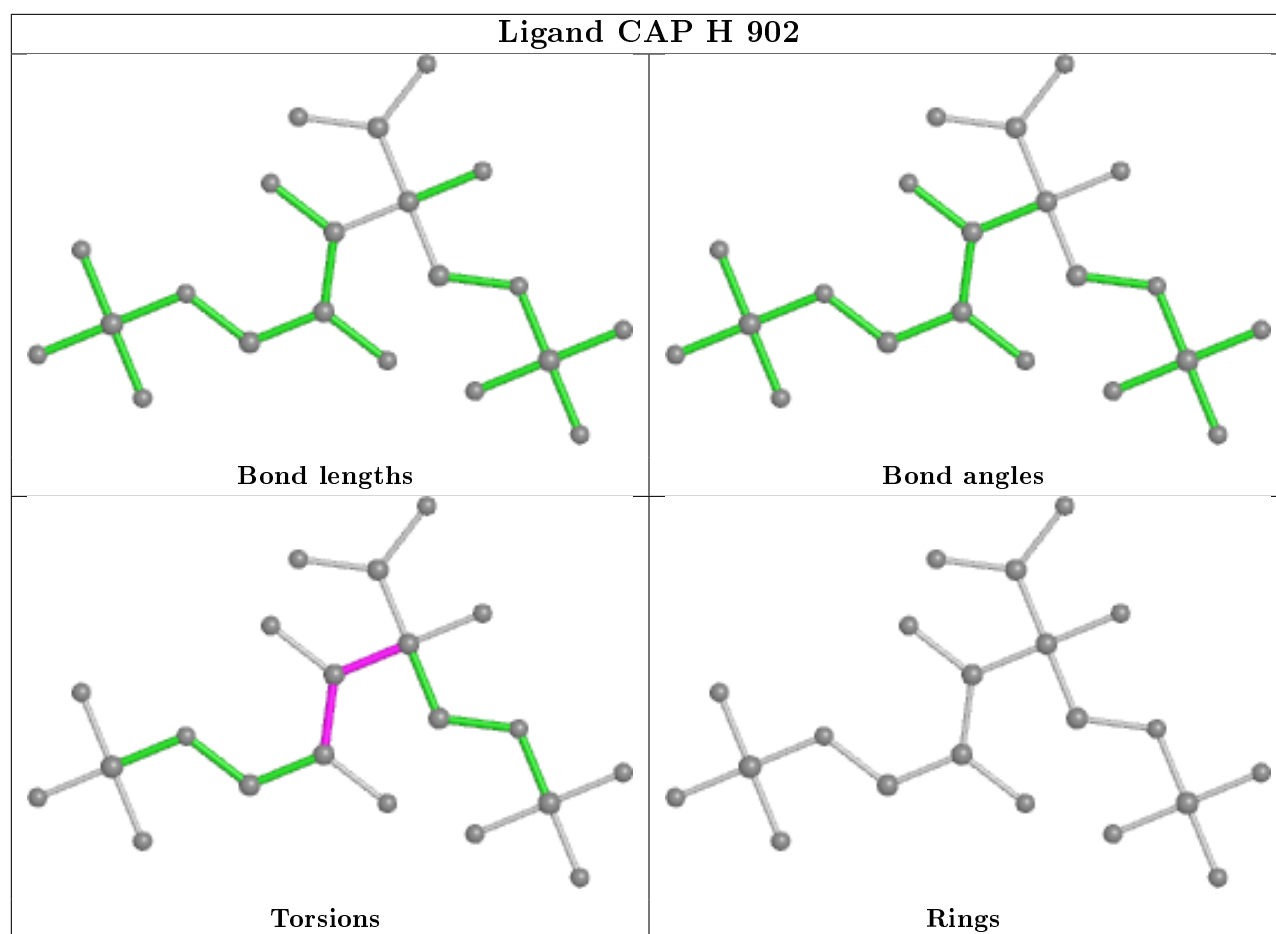












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	473/490 (96%)	-0.95	0 <span>100</span> <span>100</span>	5, 11, 23, 55	0
1	B	472/490 (96%)	-0.94	0 <span>100</span> <span>100</span>	6, 11, 23, 42	0
1	C	472/490 (96%)	-0.99	1 (0%) <span>95</span> <span>95</span>	4, 10, 20, 37	0
1	D	474/490 (96%)	-1.00	0 <span>100</span> <span>100</span>	5, 10, 22, 51	0
1	E	473/490 (96%)	-0.97	0 <span>100</span> <span>100</span>	5, 10, 23, 54	0
1	F	473/490 (96%)	-0.98	0 <span>100</span> <span>100</span>	5, 10, 23, 45	0
1	G	473/490 (96%)	-1.00	0 <span>100</span> <span>100</span>	5, 10, 21, 41	0
1	H	473/490 (96%)	-0.99	1 (0%) <span>95</span> <span>95</span>	5, 10, 21, 36	0
2	I	139/139 (100%)	-0.98	0 <span>100</span> <span>100</span>	6, 13, 23, 36	0
2	J	139/139 (100%)	-0.93	0 <span>100</span> <span>100</span>	7, 13, 22, 39	0
2	K	139/139 (100%)	-0.92	0 <span>100</span> <span>100</span>	7, 13, 22, 37	0
2	L	139/139 (100%)	-0.93	0 <span>100</span> <span>100</span>	6, 12, 23, 39	0
2	M	139/139 (100%)	-0.92	0 <span>100</span> <span>100</span>	6, 12, 23, 37	0
2	N	139/139 (100%)	-0.96	0 <span>100</span> <span>100</span>	7, 13, 22, 37	0
2	O	139/139 (100%)	-0.94	0 <span>100</span> <span>100</span>	7, 13, 22, 37	0
2	P	139/139 (100%)	-0.93	0 <span>100</span> <span>100</span>	6, 13, 23, 37	0
All	All	4895/5032 (97%)	-0.97	2 (0%) <span>100</span> <span>100</span>	4, 11, 23, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	98	THR	2.9
1	C	98	THR	2.3

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

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
1	HYP	D	48	8/9	0.95	0.09	8,10,15,27	0
1	HYP	G	48	8/9	0.95	0.08	9,10,16,23	0
1	HYP	A	48	8/9	0.96	0.06	10,13,15,19	0
1	HLU	H	174	9/10	0.96	0.07	9,10,15,16	0
1	HYP	B	48	8/9	0.96	0.07	9,14,16,21	0
1	HYP	F	48	8/9	0.96	0.07	9,11,19,20	0
1	HLU	F	174	9/10	0.96	0.08	7,11,15,17	0
1	HLU	C	174	9/10	0.96	0.07	9,10,16,16	0
1	HLU	B	174	9/10	0.96	0.09	9,13,16,18	0
1	HLU	E	174	9/10	0.96	0.08	7,11,15,16	0
1	HYP	C	48	8/9	0.97	0.06	7,10,12,15	0
1	HYP	H	48	8/9	0.97	0.06	8,10,12,17	0
1	HLU	A	174	9/10	0.97	0.07	9,12,16,17	0
1	LYO	H	198	10/11	0.97	0.07	6,10,17,20	0
1	LYO	D	150	10/11	0.97	0.06	4,8,15,18	0
1	LYO	B	150	10/11	0.97	0.07	6,7,17,20	0
1	HYP	B	155	8/9	0.97	0.06	7,8,10,11	0
1	M3L	D	346	12/13	0.97	0.06	7,12,21,22	0
1	HLU	D	174	9/10	0.97	0.09	5,9,14,15	0
1	HYP	E	48	8/9	0.97	0.07	10,11,18,21	0
1	M3L	B	346	12/13	0.97	0.07	10,17,26,27	0
1	LYO	G	198	10/11	0.98	0.07	6,12,21,22	0
1	LYO	F	150	10/11	0.98	0.07	6,7,13,16	0
1	M3L	G	346	12/13	0.98	0.06	7,14,19,20	0
1	LYO	C	198	10/11	0.98	0.06	6,11,17,18	0
1	LYO	D	198	10/11	0.98	0.07	5,11,22,26	0
1	M3L	H	346	12/13	0.98	0.07	8,14,21,21	0
1	HLU	G	174	9/10	0.98	0.07	7,10,14,15	0
1	HYP	E	155	8/9	0.98	0.05	5,7,9,11	0
1	CSO	C	109	7/8	0.98	0.06	7,9,11,18	0
1	KCX	A	205	12/13	0.98	0.06	7,9,11,11	0
1	LYO	A	150	10/11	0.98	0.06	6,7,14,19	0
1	LYO	C	150	10/11	0.98	0.07	5,6,15,17	0
1	LYO	A	198	10/11	0.98	0.07	6,10,21,21	0
1	HYP	A	155	8/9	0.98	0.05	7,8,10,11	0
1	M3L	C	346	12/13	0.98	0.07	8,12,21,21	0
1	KCX	B	205	12/13	0.98	0.05	8,8,10,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	D	205	12/13	0.98	0.06	6,7,9,10	0
1	M3L	F	346	12/13	0.98	0.08	8,18,25,28	0
1	LYO	H	150	10/11	0.98	0.07	4,7,17,18	0
1	M3L	A	346	12/13	0.98	0.07	11,19,24,25	0
1	LYO	F	198	10/11	0.98	0.06	6,10,17,19	0
1	M3L	E	346	12/13	0.98	0.08	9,18,23,25	0
1	LYO	G	150	10/11	0.98	0.06	5,7,16,20	0
1	CSO	A	109	7/8	0.99	0.06	9,10,11,21	0
1	HYP	C	155	8/9	0.99	0.05	5,7,8,9	0
1	CSO	D	109	7/8	0.99	0.05	7,8,12,15	0
1	LYO	E	198	10/11	0.99	0.06	7,11,18,21	0
1	HYP	G	155	8/9	0.99	0.05	5,8,9,10	0
1	HYP	F	155	8/9	0.99	0.05	6,7,9,10	0
1	KCX	F	205	12/13	0.99	0.05	6,8,10,10	0
1	LYO	E	150	10/11	0.99	0.06	5,7,13,18	0
1	LYO	B	198	10/11	0.99	0.06	7,11,19,22	0
1	CSO	G	109	7/8	0.99	0.05	6,8,12,17	0
1	CSO	B	109	7/8	0.99	0.06	9,9,12,20	0
1	CSO	E	109	7/8	0.99	0.04	7,8,11,16	0
1	HYP	H	155	8/9	0.99	0.05	4,7,8,8	0
1	KCX	E	205	12/13	0.99	0.05	6,8,9,10	0
1	CSO	H	109	7/8	0.99	0.05	7,8,10,17	0
1	HYP	D	155	8/9	0.99	0.04	6,8,9,9	0
1	CSO	F	109	7/8	0.99	0.05	8,8,10,17	0
1	KCX	H	205	12/13	0.99	0.05	5,8,9,9	0
1	KCX	G	205	12/13	0.99	0.05	6,7,9,9	0
1	KCX	C	205	12/13	0.99	0.05	7,8,9,9	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	I	205	4/4	0.84	0.17	26,28,30,42	0

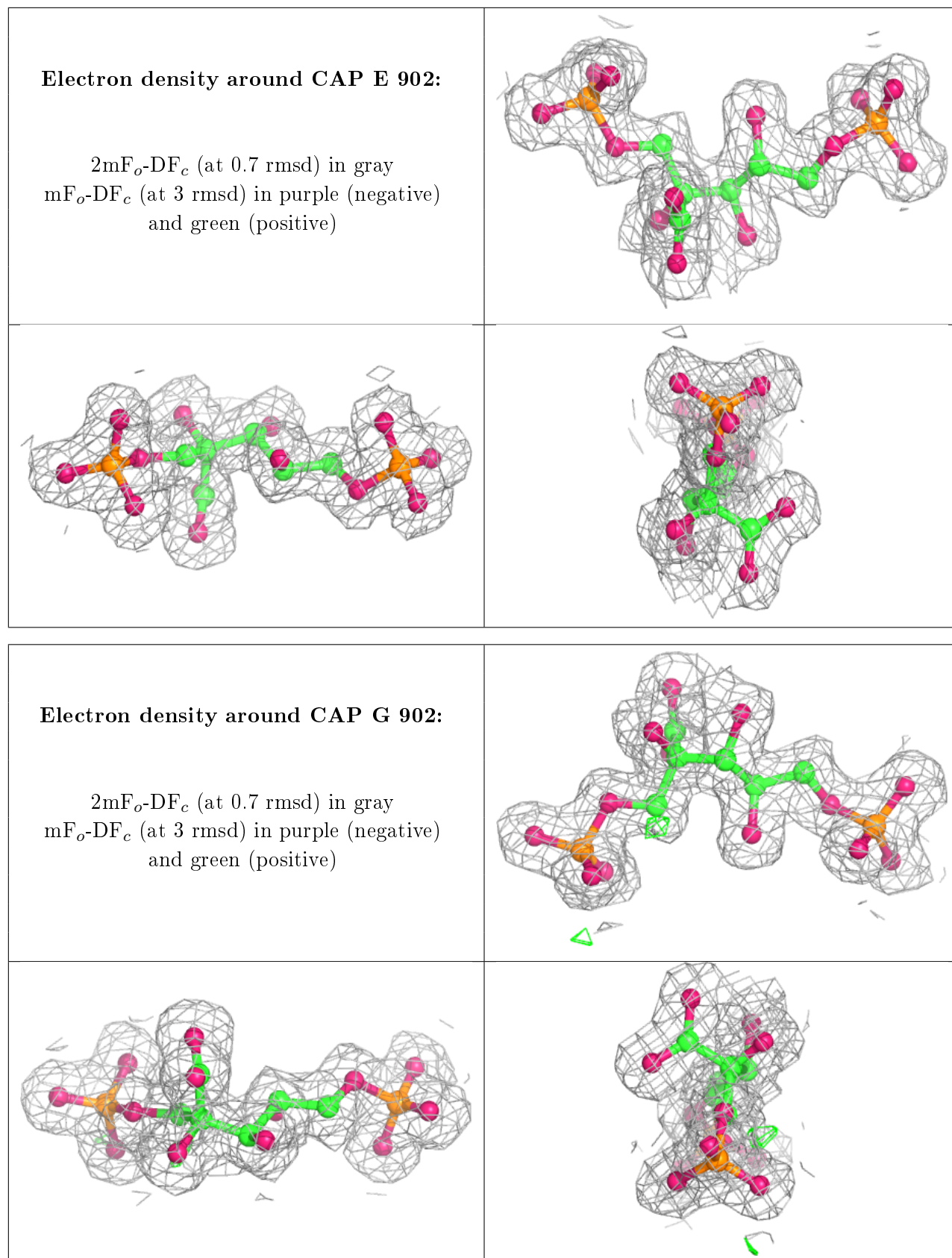
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	M	204	4/4	0.87	0.13	26,32,34,35	0
5	EDO	I	203	4/4	0.93	0.08	23,31,35,40	0
5	EDO	J	202	4/4	0.94	0.11	23,28,35,36	0
5	EDO	I	204	4/4	0.98	0.07	9,10,11,12	0
5	EDO	O	202	4/4	0.98	0.06	7,8,10,12	0
5	EDO	P	201	4/4	0.98	0.07	9,10,12,12	0
5	EDO	J	203	4/4	0.98	0.06	7,12,12,13	0
5	EDO	M	203	4/4	0.98	0.06	9,10,10,12	0
5	EDO	N	201	4/4	0.99	0.04	9,9,12,14	0
5	EDO	L	201	4/4	0.99	0.16	10,11,13,16	0
4	CAP	E	902	21/21	0.99	0.05	7,8,10,12	0
4	CAP	G	902	21/21	0.99	0.05	7,8,9,11	0
4	CAP	A	902	21/21	0.99	0.04	8,9,12,15	0
3	MG	C	901	1/1	0.99	0.04	9,9,9,9	0
5	EDO	O	201	4/4	0.99	0.05	8,11,12,13	0
3	MG	B	901	1/1	0.99	0.05	11,11,11,11	0
5	EDO	I	202	4/4	0.99	0.18	8,9,13,17	0
4	CAP	B	902	21/21	0.99	0.04	8,10,11,13	0
5	EDO	J	204	4/4	0.99	0.05	7,7,9,12	0
5	EDO	K	201	4/4	0.99	0.15	8,11,12,16	0
5	EDO	L	203	4/4	0.99	0.05	9,10,11,13	0
5	EDO	J	201	4/4	0.99	0.15	9,9,10,17	0
5	EDO	L	202	4/4	0.99	0.05	9,10,11,12	0
3	MG	H	901	1/1	0.99	0.04	9,9,9,9	0
5	EDO	A	903	4/4	0.99	0.05	7,9,9,10	0
4	CAP	C	902	21/21	0.99	0.05	6,8,9,12	0
4	CAP	D	902	21/21	0.99	0.04	7,8,10,11	0
4	CAP	H	902	21/21	0.99	0.05	6,8,9,12	0
4	CAP	F	902	21/21	0.99	0.05	6,8,9,12	0
3	MG	D	901	1/1	0.99	0.06	9,9,9,9	0
5	EDO	B	903	4/4	0.99	0.06	8,9,9,10	0
5	EDO	M	202	4/4	0.99	0.14	7,9,9,13	0
5	EDO	F	903	4/4	1.00	0.16	8,9,9,9	0
3	MG	I	201	1/1	1.00	0.13	10,10,10,10	0
3	MG	A	901	1/1	1.00	0.05	10,10,10,10	0
3	MG	F	901	1/1	1.00	0.04	8,8,8,8	0
3	MG	G	901	1/1	1.00	0.05	9,9,9,9	0
3	MG	M	201	1/1	1.00	0.13	10,10,10,10	0
3	MG	E	901	1/1	1.00	0.04	8,8,8,8	0

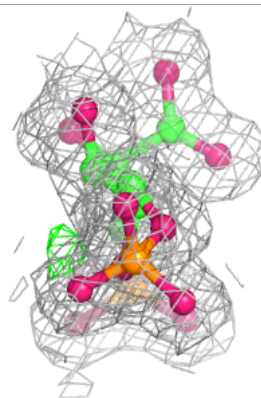
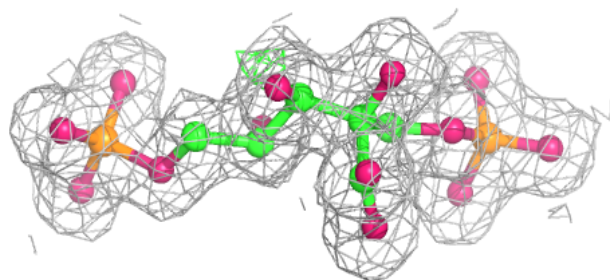
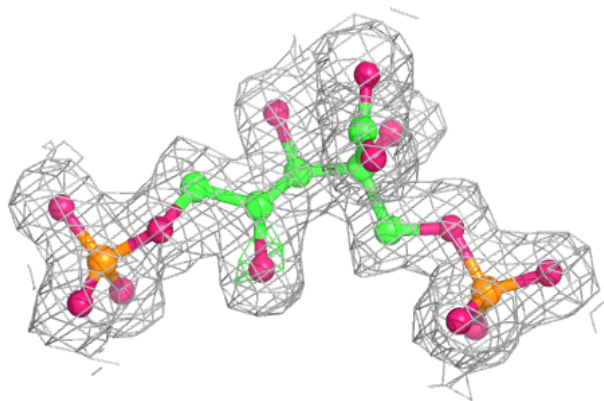
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

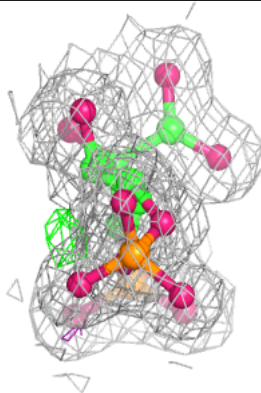
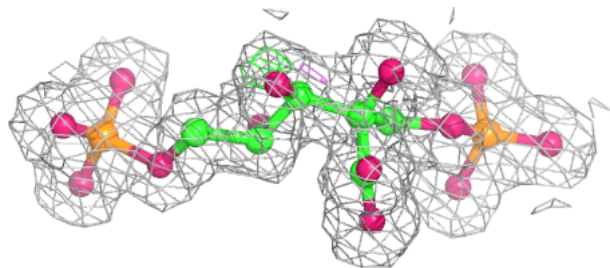
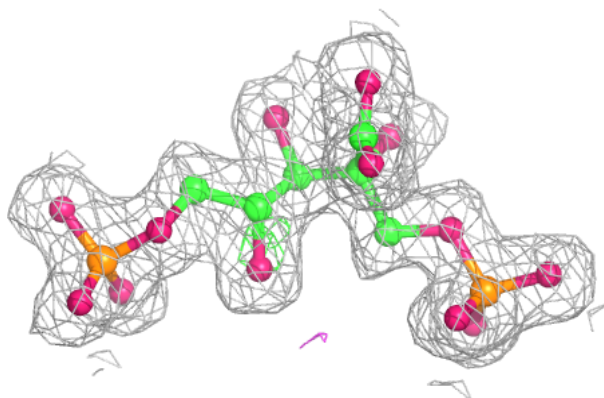


**Electron density around CAP A 902:**

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

**Electron density around CAP B 902:**

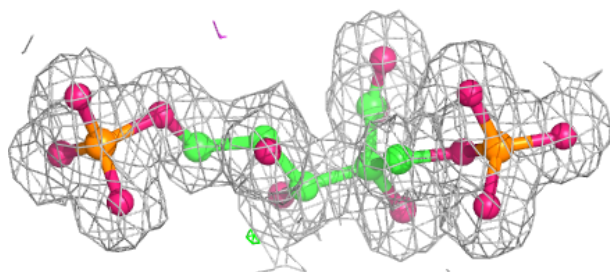
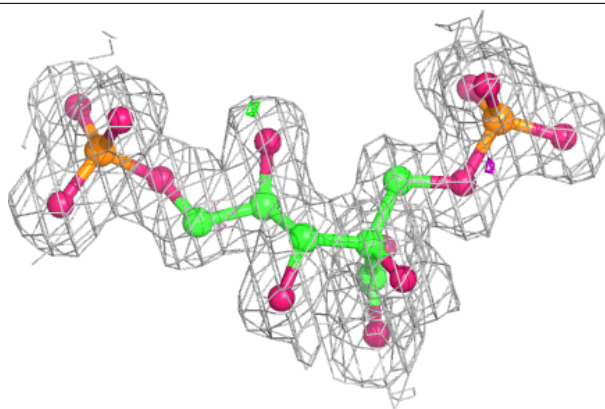
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



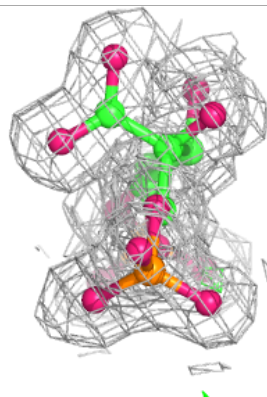
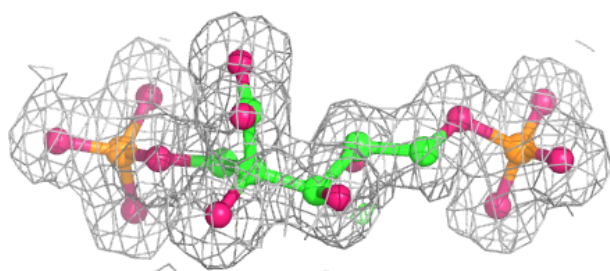
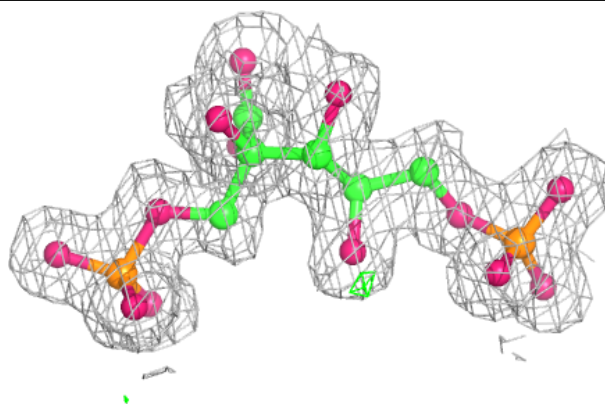


**Electron density around CAP C 902:**

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

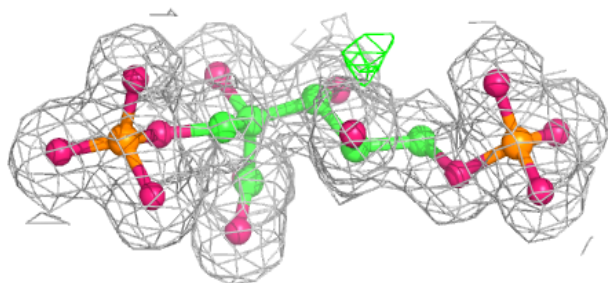
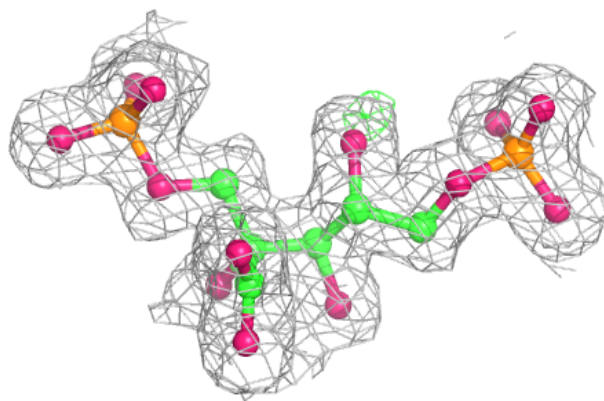
**Electron density around CAP D 902:**

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

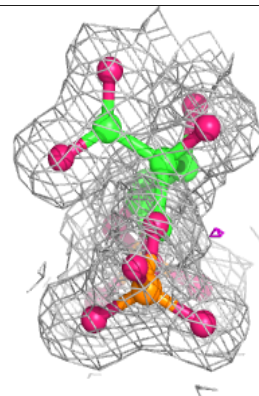
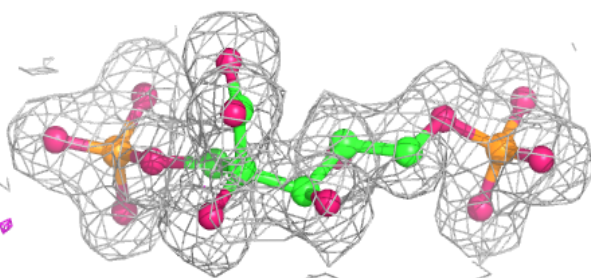
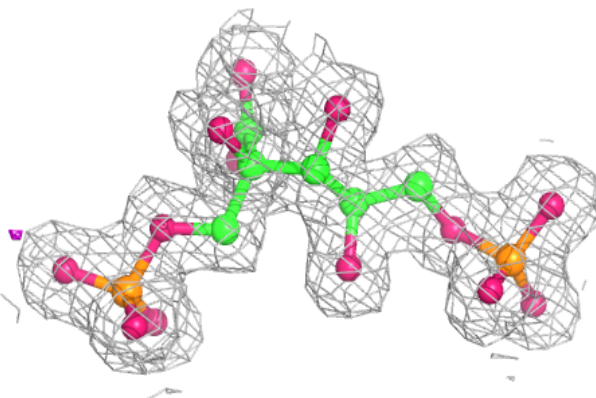


**Electron density around CAP H 902:**

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

**Electron density around CAP F 902:**

$2mF_o-DF_c$  (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.