



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:35 pm BST

PDB ID : 2V6A  
Title : Crystal structure of Chlamydomonas reinhardtii Rubisco with large- subunit mutations V331A, G344S  
Authors : Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.  
Deposited on : 2007-07-14  
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

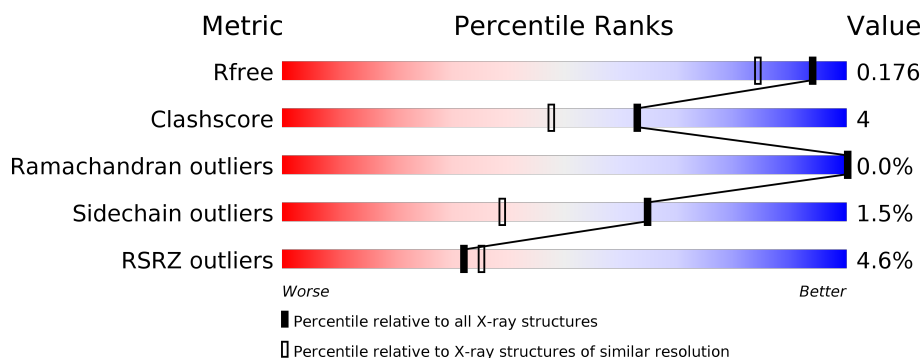
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

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





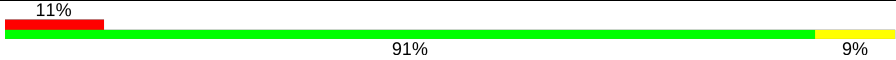
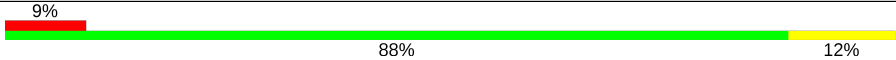
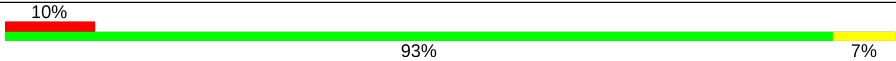
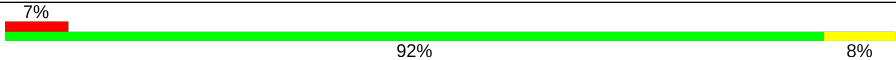
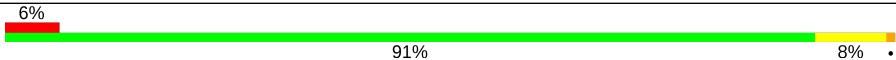
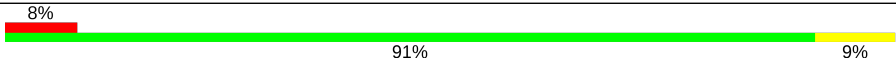
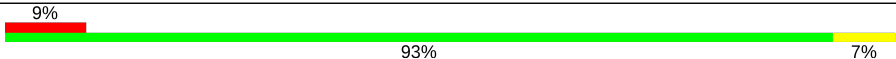
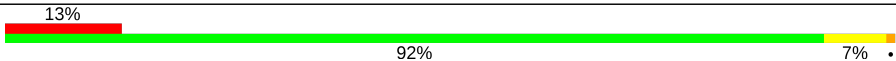
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	475	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	B	475	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	C	475	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	D	475	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	E	475	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	F	475	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	475	
1	H	475	
2	I	140	
2	J	140	
2	K	140	
2	L	140	
2	M	140	
2	N	140	
2	O	140	
2	P	140	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42413 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	9	0
			3658	2309	640	680	29			
1	B	467	Total	C	N	O	S	0	9	0
			3658	2309	640	680	29			
1	C	467	Total	C	N	O	S	0	8	0
			3655	2306	640	680	29			
1	D	466	Total	C	N	O	S	0	10	0
			3656	2307	639	681	29			
1	E	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	F	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	G	465	Total	C	N	O	S	0	9	0
			3648	2303	638	678	29			
1	H	467	Total	C	N	O	S	0	11	0
			3664	2313	640	682	29			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
A	331	ALA	VAL	engineered mutation	UNP P00877
A	344	SER	GLY	engineered mutation	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
B	331	ALA	VAL	engineered mutation	UNP P00877
B	344	SER	GLY	engineered mutation	UNP P00877
C	46	PRO	LEU	conflict	UNP P00877
C	331	ALA	VAL	engineered mutation	UNP P00877
C	344	SER	GLY	engineered mutation	UNP P00877
D	46	PRO	LEU	conflict	UNP P00877
D	331	ALA	VAL	engineered mutation	UNP P00877
D	344	SER	GLY	engineered mutation	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
E	46	PRO	LEU	conflict	UNP P00877
E	331	ALA	VAL	engineered mutation	UNP P00877
E	344	SER	GLY	engineered mutation	UNP P00877
F	46	PRO	LEU	conflict	UNP P00877
F	331	ALA	VAL	engineered mutation	UNP P00877
F	344	SER	GLY	engineered mutation	UNP P00877
G	46	PRO	LEU	conflict	UNP P00877
G	331	ALA	VAL	engineered mutation	UNP P00877
G	344	SER	GLY	engineered mutation	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
H	331	ALA	VAL	engineered mutation	UNP P00877
H	344	SER	GLY	engineered mutation	UNP P00877

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	3	0
			1147	740	190	205	12			
2	J	140	Total	C	N	O	S	0	4	0
			1155	747	190	206	12			
2	K	140	Total	C	N	O	S	0	5	0
			1162	753	190	207	12			
2	L	140	Total	C	N	O	S	0	6	0
			1163	754	190	206	13			
2	M	140	Total	C	N	O	S	0	6	0
			1164	754	190	207	13			
2	N	140	Total	C	N	O	S	0	5	0
			1163	754	190	206	13			
2	O	140	Total	C	N	O	S	0	6	0
			1158	748	190	206	14			
2	P	140	Total	C	N	O	S	0	5	0
			1162	753	190	207	12			

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

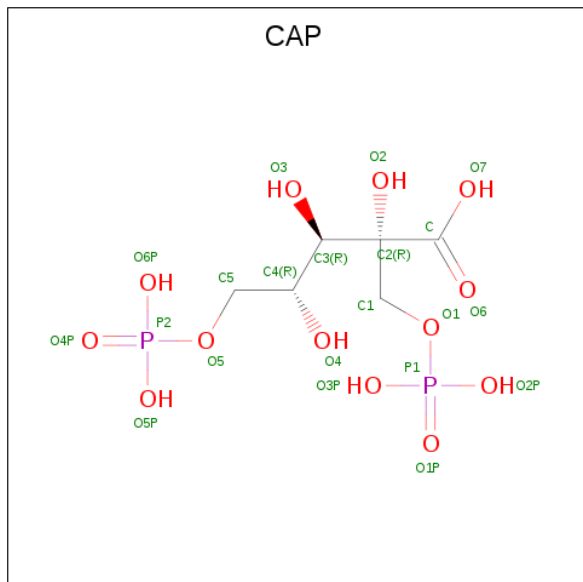
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	B	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		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



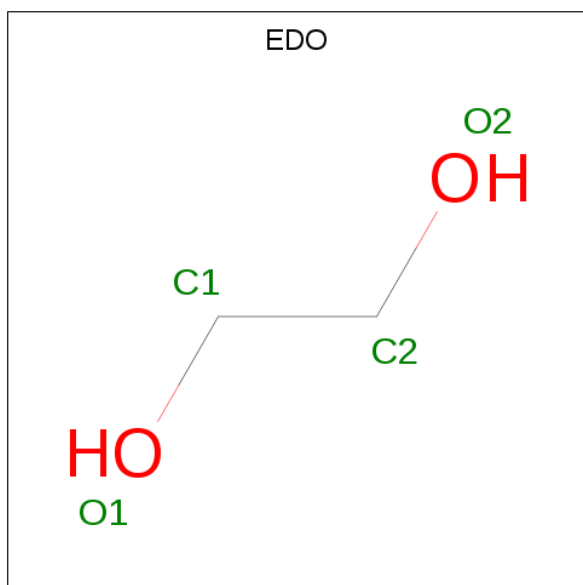
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	I	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
5	K	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0
5	L	1	Total 4	C 2	O 2	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	327	Total O 327 327	0	0
6	B	334	Total O 334 334	0	0
6	C	320	Total O 320 320	0	0
6	D	332	Total O 332 332	0	0
6	E	344	Total O 344 344	0	0
6	F	330	Total O 330 330	0	0
6	G	324	Total O 324 324	0	0
6	H	330	Total O 330 330	0	0
6	I	97	Total O 97 97	0	0
6	J	106	Total O 106 106	0	0
6	K	100	Total O 100 100	0	0

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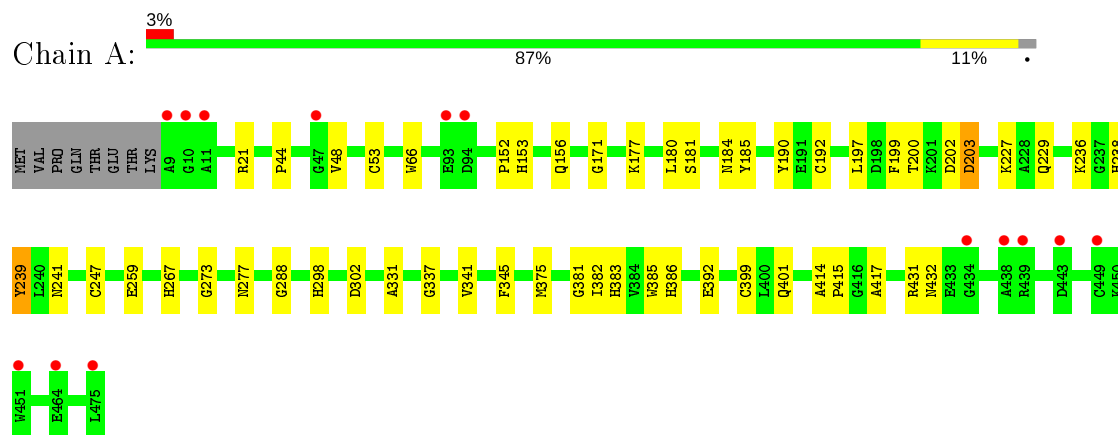
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	111	Total 111	O 111	0	0
6	M	112	Total 112	O 112	0	0
6	N	111	Total 111	O 111	0	0
6	O	114	Total 114	O 114	0	0
6	P	100	Total 100	O 100	0	0

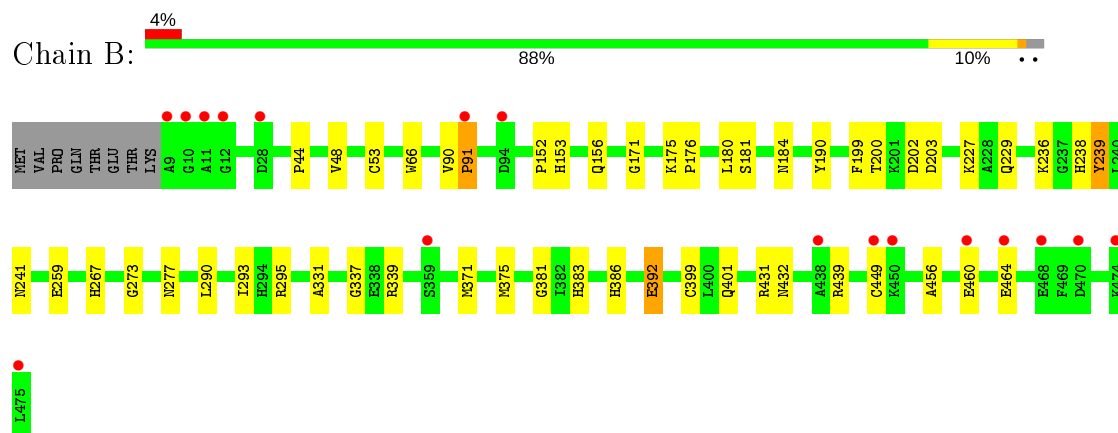
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

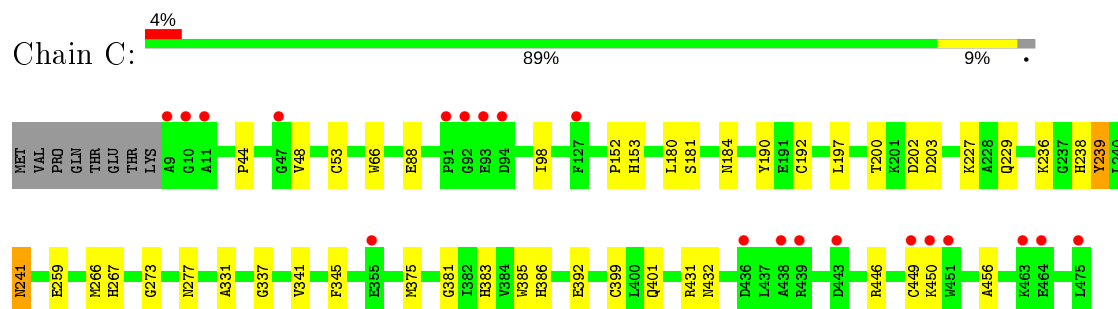
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



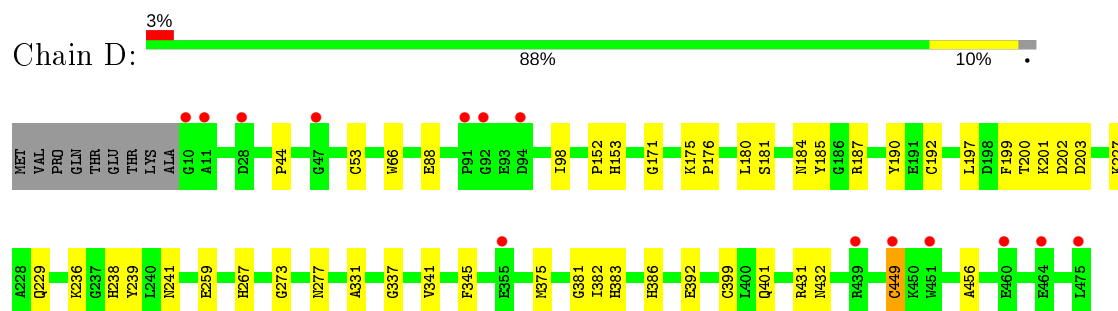
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



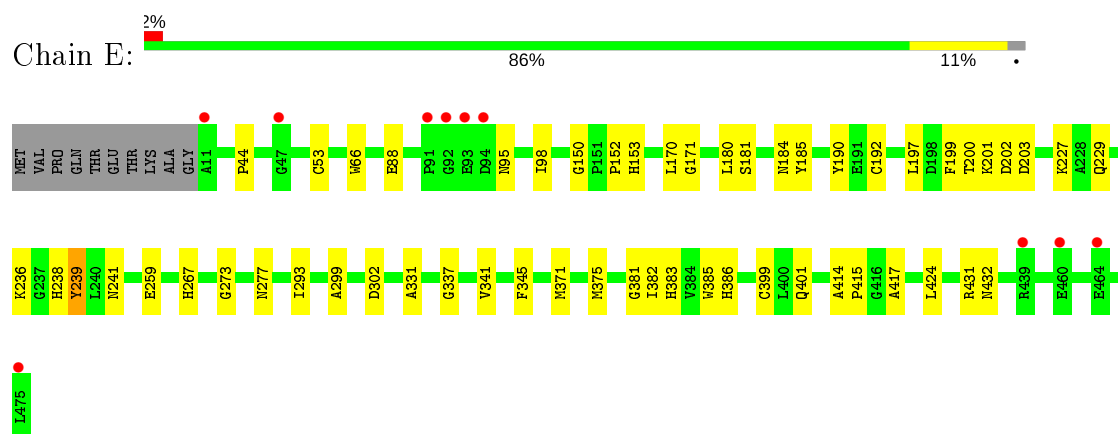
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



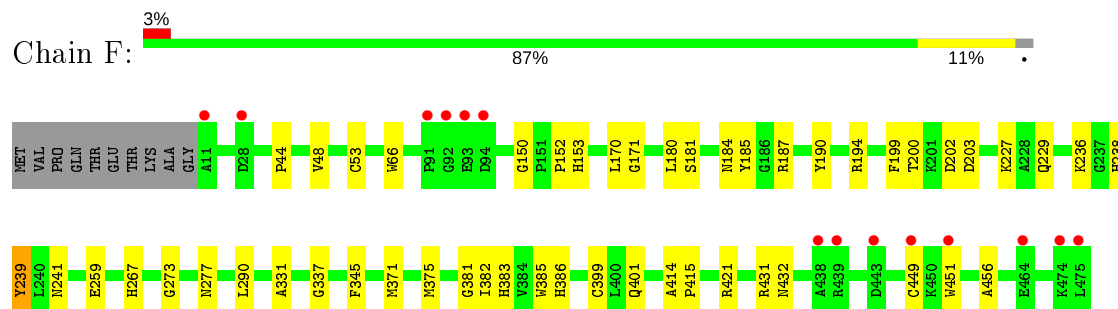
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



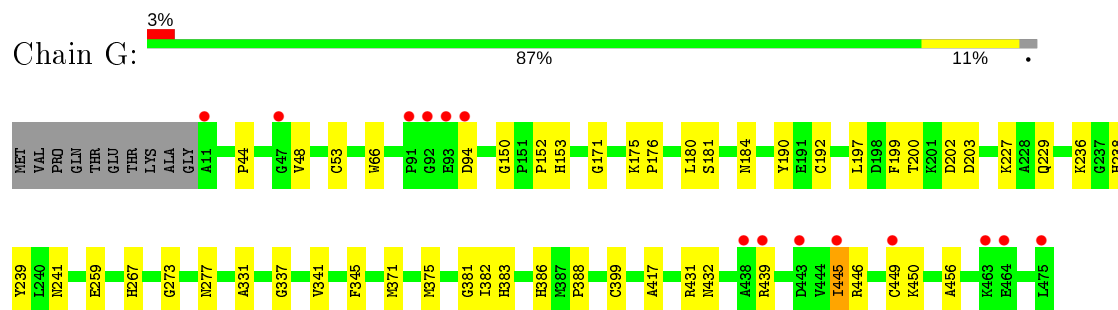
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



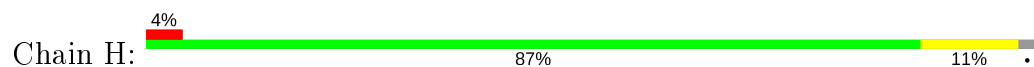
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

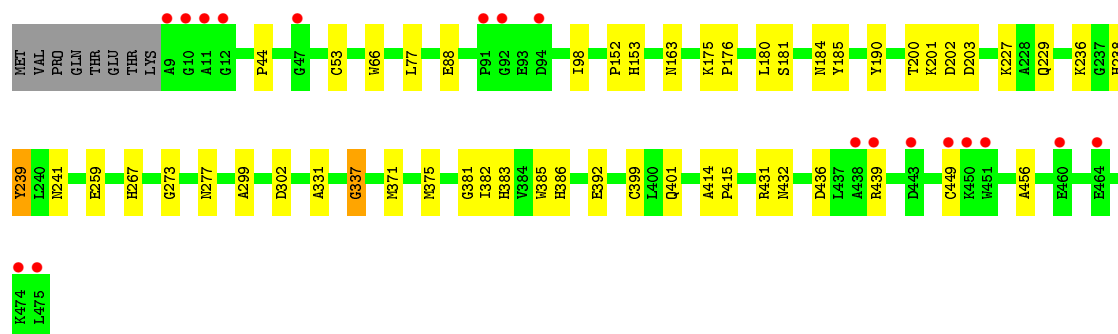


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

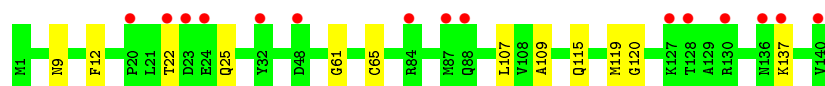


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

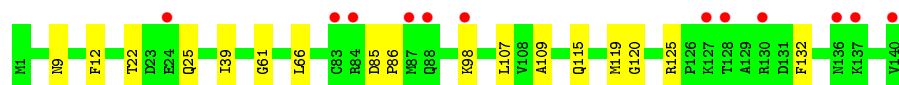
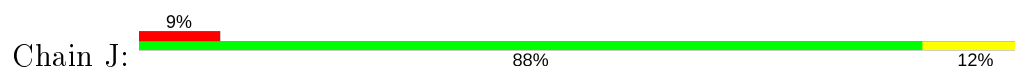




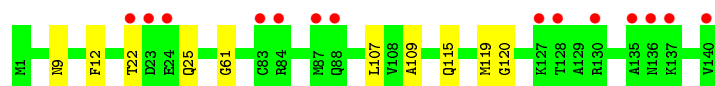
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



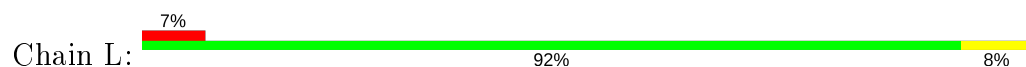
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



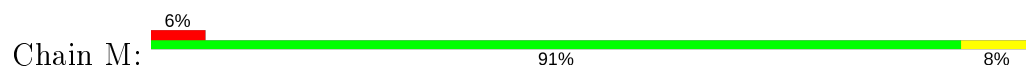
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

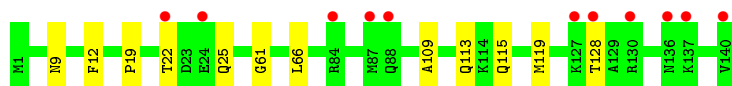


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

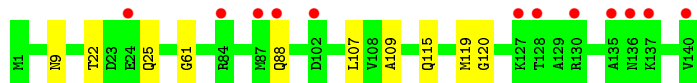


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

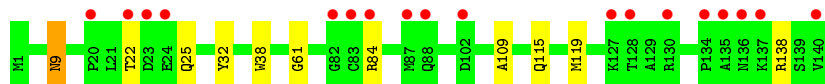




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.91Å 196.63Å 201.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 14.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-1.50) 95.8 (14.99-1.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.192 0.175 , 0.176	Depositor DCC
$R_{free}$ test set	39010 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	42413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, EDO, HYP, MME, SMC, 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	0.50	0/3743	0.65	0/5059
1	B	0.49	0/3743	0.64	0/5059
1	C	0.50	0/3735	0.64	0/5048
1	D	0.51	0/3747	0.65	2/5064 (0.0%)
1	E	0.50	0/3734	0.65	0/5047
1	F	0.51	0/3734	0.65	1/5047 (0.0%)
1	G	0.51	0/3734	0.66	0/5047
1	H	0.52	0/3758	0.65	0/5080
2	I	0.47	0/1184	0.60	0/1608
2	J	0.48	0/1197	0.62	0/1626
2	K	0.48	0/1210	0.62	0/1644
2	L	0.48	0/1217	0.62	0/1654
2	M	0.46	0/1218	0.62	0/1654
2	N	0.47	0/1212	0.60	0/1646
2	O	0.47	0/1213	0.62	0/1646
2	P	0.49	0/1210	0.61	0/1644
All	All	0.50	0/39589	0.64	3/53573 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	D	187	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	D	449	CYS	CA-CB-SG	5.05	123.08	114.00

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	3658	0	3556	43	0
1	B	3658	0	3556	36	0
1	C	3655	0	3551	34	0
1	D	3656	0	3551	34	0
1	E	3648	0	3548	41	0
1	F	3648	0	3546	39	0
1	G	3648	0	3546	35	0
1	H	3664	0	3563	38	0
2	I	1147	0	1125	9	0
2	J	1155	0	1130	12	0
2	K	1162	0	1135	8	0
2	L	1163	0	1136	8	0
2	M	1164	0	1136	9	0
2	N	1163	0	1135	11	0
2	O	1158	0	1132	8	0
2	P	1162	0	1135	8	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
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	7	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	7	0	0
4	H	21	0	7	0	0
5	A	28	0	42	0	0
5	B	20	0	30	1	0
5	C	24	0	36	0	0
5	D	20	0	30	0	0
5	E	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	24	0	36	1	0
5	G	20	0	30	0	0
5	H	20	0	30	0	0
5	I	8	0	12	0	0
5	J	8	0	12	0	0
5	K	8	0	12	0	0
5	L	8	0	12	0	0
5	M	8	0	12	0	0
5	N	8	0	12	0	0
5	O	8	0	12	0	0
5	P	8	0	12	0	0
6	A	327	0	0	3	0
6	B	334	0	0	3	0
6	C	320	0	0	1	0
6	D	332	0	0	3	0
6	E	344	0	0	3	0
6	F	330	0	0	3	0
6	G	324	0	0	3	0
6	H	330	0	0	3	0
6	I	97	0	0	0	0
6	J	106	0	0	0	0
6	K	100	0	0	0	0
6	L	111	0	0	0	0
6	M	112	0	0	2	0
6	N	111	0	0	2	0
6	O	114	0	0	0	0
6	P	100	0	0	0	0
All	All	42413	0	37891	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.01	0.99
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.01	0.99
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.02	0.99
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.05	0.98
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.02	0.97
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.02	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375[B]:MET:SD	1:G:399[B]:CYS:SG	2.63	0.96
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.03	0.95
1:D:184:ASN:HD22	2:N:115:GLN:HE21	1.14	0.95
1:G:184:ASN:HD22	2:M:115:GLN:HE21	1.14	0.94
1:H:371[B]:MET:SD	6:H:1127:HOH:O	2.25	0.94
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.06	0.93
1:H:184:ASN:HD22	2:J:115:GLN:HE21	1.16	0.92
1:C:184:ASN:HD22	2:I:115:GLN:HE21	1.18	0.90
1:F:184:ASN:HD22	2:P:115:GLN:HE21	1.19	0.89
1:E:184:ASN:HD22	2:K:115:GLN:HE21	1.18	0.88
1:A:184:ASN:HD22	2:O:115:GLN:HE21	1.16	0.88
1:F:371[B]:MET:SD	6:F:1122:HOH:O	2.32	0.87
1:C:375[B]:MET:SD	1:C:399[B]:CYS:SG	2.74	0.86
1:F:267:HIS:CD2	1:F:277:ASN:HD22	1.92	0.86
1:A:375[B]:MET:SD	1:A:399[B]:CYS:SG	2.73	0.85
1:B:184:ASN:HD22	2:L:115:GLN:HE21	1.21	0.85
1:D:267:HIS:CD2	1:D:277:ASN:HD22	1.94	0.84
1:G:267:HIS:CD2	1:G:277:ASN:HD22	1.93	0.84
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.96	0.83
1:D:375[B]:MET:SD	1:D:399[B]:CYS:SG	2.76	0.83
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.94	0.83
1:E:375[B]:MET:SD	1:E:399[B]:CYS:SG	2.77	0.82
1:D:383:HIS:H	1:D:386:HIS:HD2	1.27	0.82
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.94	0.81
1:F:375[B]:MET:SD	1:F:399[B]:CYS:SG	2.79	0.81
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.28	0.80
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.94	0.79
1:E:383:HIS:H	1:E:386:HIS:HD2	1.28	0.79
1:H:383:HIS:H	1:H:386:HIS:HD2	1.29	0.79
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.30	0.79
1:B:383:HIS:H	1:B:386:HIS:HD2	1.30	0.79
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.29	0.78
1:D:431:ARG:HH21	1:D:432:ASN:HD21	1.28	0.78
1:C:383:HIS:H	1:C:386:HIS:HD2	1.32	0.77
1:C:267:HIS:CD2	1:C:277:ASN:HD22	1.97	0.77
1:F:44:PRO:HB3	1:F:53[B]:CYS:SG	2.25	0.76
1:F:431:ARG:HH21	1:F:432:ASN:HD21	1.33	0.76
1:H:44:PRO:HB3	1:H:53[B]:CYS:SG	2.26	0.75
1:B:375[B]:MET:SD	1:B:399[B]:CYS:SG	2.83	0.75
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.33	0.75
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:PRO:HB3	1:G:53[B]:CYS:SG	2.28	0.74
2:J:22:THR:H	2:J:25:GLN:HE21	1.36	0.73
2:O:22:THR:H	2:O:25:GLN:HE21	1.34	0.72
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.37	0.72
1:D:44:PRO:HB3	1:D:53[B]:CYS:SG	2.29	0.72
1:F:383:HIS:H	1:F:386:HIS:HD2	1.38	0.72
1:A:383:HIS:H	1:A:386:HIS:HD2	1.34	0.72
1:E:44:PRO:HB3	1:E:53[B]:CYS:SG	2.30	0.71
2:N:22:THR:H	2:N:25:GLN:HE21	1.38	0.71
1:C:44:PRO:HB3	1:C:53[B]:CYS:SG	2.30	0.70
1:A:44:PRO:HB3	1:A:53[B]:CYS:SG	2.31	0.70
1:H:375[B]:MET:SD	1:H:399[B]:CYS:SG	2.90	0.70
1:G:383:HIS:H	1:G:386:HIS:HD2	1.40	0.70
2:I:22:THR:H	2:I:25:GLN:HE21	1.37	0.70
1:E:371[B]:MET:SD	6:E:1120:HOH:O	2.51	0.69
2:L:22:THR:H	2:L:25:GLN:HE21	1.40	0.68
2:M:22:THR:H	2:M:25:GLN:HE21	1.41	0.68
1:B:44:PRO:HB3	1:B:53[B]:CYS:SG	2.34	0.68
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.77	0.67
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.77	0.67
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.78	0.67
1:E:383:HIS:H	1:E:386:HIS:CD2	2.13	0.66
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.80	0.65
2:P:22:THR:H	2:P:25:GLN:HE21	1.44	0.65
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.79	0.64
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.81	0.64
2:K:22:THR:H	2:K:25:GLN:HE21	1.43	0.64
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.81	0.64
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.79	0.64
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.82	0.63
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.82	0.61
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.82	0.61
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.83	0.61
2:P:9:ASN:HD21	2:P:138:ARG:HG2	1.65	0.61
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.82	0.61
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.84	0.61
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.49	0.61
1:H:383:HIS:H	1:H:386:HIS:CD2	2.16	0.61
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.84	0.61
1:G:331:ALA:HA	1:G:337:GLY:O	2.01	0.61
1:E:331:ALA:HA	1:E:337:GLY:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:HA	1:C:337:GLY:O	2.00	0.60
2:J:109:ALA:HB3	2:J:119:MET:HG3	1.83	0.60
1:G:439:ARG:NH1	6:G:1285:HOH:O	2.35	0.60
1:D:331:ALA:HA	1:D:337:GLY:O	2.02	0.59
2:O:109:ALA:HB3	2:O:119:MET:HG3	1.85	0.59
1:A:383:HIS:H	1:A:386:HIS:CD2	2.19	0.59
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.86	0.59
1:B:331:ALA:HA	1:B:337:GLY:O	2.03	0.59
1:A:331:ALA:HA	1:A:337:GLY:O	2.03	0.58
1:C:383:HIS:H	1:C:386:HIS:CD2	2.17	0.58
1:F:331:ALA:HA	1:F:337:GLY:O	2.04	0.58
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.52	0.58
1:G:383:HIS:H	1:G:386:HIS:CD2	2.21	0.58
1:C:88:GLU:HG3	1:C:98:ILE:HB	1.86	0.58
1:H:88:GLU:HG2	1:H:98:ILE:HB	1.84	0.58
1:E:88:GLU:HG3	1:E:98:ILE:HB	1.86	0.57
1:D:181:SER:H	2:N:115:GLN:NE2	2.03	0.57
1:B:383:HIS:H	1:B:386:HIS:CD2	2.18	0.56
1:H:331:ALA:HA	1:H:337:GLY:O	2.06	0.56
1:D:383:HIS:H	1:D:386:HIS:CD2	2.16	0.56
2:M:109:ALA:HB3	2:M:119:MET:HG3	1.87	0.56
1:E:229:GLN:HE21	1:E:236:LYS:H	1.54	0.56
1:G:192:CYS:HB3	1:G:197:LEU:HD12	1.88	0.56
1:F:383:HIS:H	1:F:386:HIS:CD2	2.22	0.55
1:C:181:SER:H	2:I:115:GLN:NE2	2.05	0.55
1:F:180:LEU:HA	2:P:115:GLN:HE22	1.72	0.54
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.54	0.54
2:O:22:THR:H	2:O:25:GLN:NE2	2.04	0.54
1:G:446:ARG:O	1:G:450:LYS:HG3	2.06	0.54
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.55	0.54
1:H:431:ARG:HE	1:H:432:ASN:HD22	1.55	0.54
2:M:125:ARG:HD2	6:M:1097:HOH:O	2.06	0.54
2:L:109:ALA:HB3	2:L:119:MET:HG3	1.90	0.53
2:I:109:ALA:HB3	2:I:119:MET:HG3	1.90	0.53
1:C:48:VAL:CG1	1:C:53[B]:CYS:SG	2.96	0.53
1:D:259[B]:GLU:OE1	2:N:61:GLY:HA3	2.08	0.53
1:H:181:SER:H	2:J:115:GLN:NE2	2.07	0.53
6:E:1204:HOH:O	1:F:267:HIS:HE1	1.90	0.53
1:B:181:SER:H	2:L:115:GLN:NE2	2.07	0.53
1:A:229:GLN:HE21	1:A:236:LYS:H	1.57	0.53
1:C:267:HIS:HE1	6:D:1198:HOH:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.86	0.53
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.57	0.53
1:D:88:GLU:HG2	1:D:98:ILE:HB	1.89	0.53
1:G:181:SER:H	2:M:115:GLN:NE2	2.06	0.53
1:C:229:GLN:HE21	1:C:236:LYS:H	1.57	0.52
1:A:181:SER:H	2:O:115:GLN:NE2	2.06	0.52
1:F:181:SER:H	2:P:115:GLN:NE2	2.08	0.52
6:C:1192:HOH:O	1:D:267:HIS:HE1	1.93	0.52
1:E:181:SER:H	2:K:115:GLN:NE2	2.07	0.52
1:E:180:LEU:HA	2:K:115:GLN:HE22	1.74	0.51
1:H:229:GLN:HE21	1:H:236:LYS:H	1.59	0.51
1:B:180:LEU:HA	2:L:115:GLN:HE22	1.76	0.51
1:A:288:GLY:O	2:I:65[B]:CYS:SG	2.64	0.50
6:G:1190:HOH:O	1:H:267:HIS:HE1	1.93	0.50
1:H:180:LEU:HA	2:J:115:GLN:HE22	1.76	0.50
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.47	0.50
1:A:180:LEU:HA	2:O:115:GLN:HE22	1.77	0.50
1:A:48:VAL:CG1	1:A:53[B]:CYS:SG	3.00	0.50
1:D:229:GLN:HE21	1:D:236:LYS:H	1.60	0.50
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.09	0.50
1:C:48:VAL:HG12	1:C:53[B]:CYS:SG	2.51	0.50
1:E:201:KCX:HB2	1:E:239:TYR:CD2	2.46	0.49
1:G:180:LEU:HA	2:M:115:GLN:HE22	1.75	0.49
1:B:290:LEU:HG	2:J:66:LEU:HD11	1.95	0.49
1:C:180:LEU:HA	2:I:115:GLN:HE22	1.77	0.49
2:K:22:THR:H	2:K:25:GLN:NE2	2.09	0.49
1:F:259[B]:GLU:OE1	2:P:61:GLY:HA3	2.12	0.49
1:A:259[B]:GLU:OE1	2:O:61:GLY:HA3	2.12	0.49
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.93	0.49
1:G:267:HIS:HE1	6:H:1208:HOH:O	1.95	0.49
6:A:1195:HOH:O	1:B:267:HIS:HE1	1.94	0.49
1:C:381:GLY:HA2	1:D:66:TRP:CD1	2.48	0.49
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.94	0.49
2:K:109:ALA:HB3	2:K:119:MET:HG3	1.95	0.49
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.60	0.48
2:J:22:THR:H	2:J:25:GLN:NE2	2.09	0.48
1:E:267:HIS:HE1	6:F:1200:HOH:O	1.97	0.48
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.48	0.48
1:G:259[B]:GLU:OE1	2:M:61:GLY:HA3	2.13	0.48
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.95	0.47
1:E:171:GLY:HA2	1:E:199:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:22:THR:H	2:N:25:GLN:NE2	2.09	0.47
1:D:383:HIS:N	1:D:386:HIS:HD2	2.04	0.47
1:G:171:GLY:HA2	1:G:199:PHE:O	2.15	0.47
2:N:109:ALA:HB3	2:N:119:MET:HG3	1.96	0.47
1:B:229:GLN:HE21	1:B:236:LYS:H	1.63	0.47
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.50	0.47
1:C:383:HIS:N	1:C:386:HIS:HD2	2.08	0.47
2:J:125:ARG:HD2	2:J:132:PHE:CE2	2.50	0.47
1:A:267:HIS:HE1	6:B:1207:HOH:O	1.98	0.46
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.50	0.46
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.97	0.46
1:D:239:TYR:HE2	1:D:401:GLN:NE2	2.14	0.46
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.96	0.46
1:G:153:HIS:HE1	6:G:1192:HOH:O	1.97	0.46
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.50	0.46
1:B:339:ARG:NH1	1:B:392:GLU:OE2	2.49	0.46
1:E:239:TYR:HE2	1:E:401:GLN:NE2	2.14	0.46
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.51	0.46
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.51	0.46
1:D:449:CYS:O	1:D:456:ALA:HB2	2.16	0.45
1:F:152:PRO:HB2	1:F:153:HIS:CD2	2.52	0.45
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.63	0.45
1:D:180:LEU:HA	2:N:115:GLN:HE22	1.81	0.45
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.99	0.45
1:B:383:HIS:N	1:B:386:HIS:HD2	2.07	0.45
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.51	0.45
1:F:150:GLY:HA3	1:F:371[B]:MET:SD	2.56	0.45
1:G:200:THR:OG1	1:G:238:HIS:CD2	2.65	0.45
1:E:259[B]:GLU:OE1	2:K:61:GLY:HA3	2.16	0.45
1:B:259[B]:GLU:OE1	2:L:61:GLY:HA3	2.16	0.45
2:P:109:ALA:HB3	2:P:119:MET:HG3	1.98	0.45
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.82	0.45
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.52	0.45
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.52	0.45
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.52	0.45
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.51	0.45
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.53	0.44
1:A:171:GLY:HA2	1:A:199:PHE:O	2.17	0.44
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.88	0.44
1:B:153:HIS:HE1	6:B:1211:HOH:O	2.00	0.44
1:E:44:PRO:O	1:E:95:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:GLY:HA2	1:H:66:TRP:CD1	2.52	0.44
1:H:77:LEU:HA	1:H:77:LEU:HD12	1.90	0.44
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.98	0.44
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.53	0.44
1:G:382:ILE:HA	1:G:386:HIS:CD2	2.53	0.44
1:G:66:TRP:CD1	1:H:381:GLY:HA2	2.53	0.44
1:F:229:GLN:HE21	1:F:236:LYS:H	1.66	0.44
1:H:299:ALA:HA	1:H:302:ASP:OD1	2.18	0.44
1:E:192:CYS:HB3	1:E:197:LEU:HD12	1.99	0.44
1:E:190:TYR:CZ	1:E:227:LYS:HE3	2.53	0.43
1:D:449:CYS:HB3	1:D:456:ALA:HA	1.99	0.43
1:H:449:CYS:O	1:H:456:ALA:HB2	2.18	0.43
1:A:383:HIS:N	1:A:386:HIS:HD2	2.09	0.43
1:F:345:PHE:HE1	5:F:1483:EDO:H21	1.83	0.43
1:H:153:HIS:HE1	6:H:1213:HOH:O	2.02	0.43
2:K:107:LEU:O	2:K:120:GLY:HA2	2.19	0.43
1:A:153:HIS:HE1	6:A:1200:HOH:O	2.01	0.43
2:M:107:LEU:O	2:M:120:GLY:HA2	2.18	0.43
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.68	0.43
1:A:273:GLY:HA3	1:B:273:GLY:HA3	2.01	0.43
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.54	0.43
1:E:383:HIS:N	1:E:386:HIS:HD2	2.05	0.43
1:G:48:VAL:CG1	1:G:53[B]:CYS:SG	3.07	0.43
1:H:175:LYS:HA	1:H:176:PRO:C	2.39	0.43
1:D:192:CYS:HB3	1:D:197:LEU:HD12	2.00	0.43
1:D:341:VAL:HG12	1:D:345:PHE:CZ	2.54	0.43
1:C:200:THR:OG1	1:C:238:HIS:CD2	2.69	0.43
1:C:239:TYR:HE2	1:C:401:GLN:NE2	2.15	0.43
1:E:299:ALA:HA	1:E:302:ASP:OD1	2.18	0.43
1:E:341:VAL:HG12	1:E:345:PHE:CZ	2.53	0.43
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.01	0.43
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.52	0.43
1:H:436:ASP:OD2	1:H:439:ARG:HD3	2.18	0.43
1:D:171:GLY:HA2	1:D:199:PHE:O	2.19	0.43
1:G:341:VAL:HG12	1:G:345:PHE:CZ	2.54	0.43
2:O:107:LEU:O	2:O:120:GLY:HA2	2.19	0.43
1:G:388:PRO:HD3	1:G:445:ILE:HG13	2.01	0.42
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.55	0.42
1:F:449:CYS:O	1:F:456:ALA:HB2	2.19	0.42
1:H:259[B]:GLU:OE1	2:J:61:GLY:HA3	2.19	0.42
1:F:382:ILE:HA	1:F:386:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.42
1:D:153:HIS:HE1	6:D:1201:HOH:O	2.02	0.42
1:G:229:GLN:HE21	1:G:236:LYS:H	1.65	0.42
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.55	0.42
2:I:22:THR:H	2:I:25:GLN:NE2	2.12	0.42
1:F:171:GLY:HA2	1:F:199:PHE:O	2.19	0.42
1:H:200:THR:OG1	1:H:238:HIS:CD2	2.67	0.42
1:B:295:ARG:HH12	5:B:1482:EDO:C1	2.32	0.42
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.55	0.42
1:C:341:VAL:HG12	1:C:345:PHE:CZ	2.54	0.42
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.54	0.42
1:G:150:GLY:HA3	1:G:371[B]:MET:SD	2.60	0.42
1:C:446:ARG:O	1:C:450:LYS:HG2	2.20	0.42
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.02	0.42
1:E:200:THR:OG1	1:E:238:HIS:CD2	2.69	0.42
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.55	0.42
2:M:113:GLN:NE2	6:M:1083:HOH:O	2.52	0.42
1:D:382:ILE:HA	1:D:386:HIS:CD2	2.55	0.42
1:F:200:THR:OG1	1:F:238:HIS:CD2	2.71	0.42
1:G:175:LYS:HA	1:G:176:PRO:C	2.40	0.42
1:A:48:VAL:HG11	1:A:53[B]:CYS:SG	2.60	0.42
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.55	0.42
1:A:341:VAL:HG12	1:A:345:PHE:CZ	2.54	0.41
1:B:48:VAL:CG1	1:B:53[B]:CYS:SG	3.08	0.41
1:C:449:CYS:O	1:C:456:ALA:HB2	2.20	0.41
1:F:383:HIS:HE1	1:F:385:TRP:HB2	1.84	0.41
1:G:273:GLY:HA3	1:H:273:GLY:HA3	2.02	0.41
1:H:201:KCX:HB2	1:H:239:TYR:CD2	2.55	0.41
1:C:273:GLY:HA3	1:D:273:GLY:HA3	2.02	0.41
1:F:153:HIS:HE1	6:F:1206:HOH:O	2.03	0.41
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.55	0.41
2:J:107:LEU:O	2:J:120:GLY:HA2	2.20	0.41
1:F:451:TRP:CE2	2:N:19:PRO:HG3	2.55	0.41
1:A:197:LEU:HG	1:A:417:ALA:HB1	2.03	0.41
2:L:107:LEU:O	2:L:120:GLY:HA2	2.20	0.41
1:F:383:HIS:N	1:F:386:HIS:HD2	2.12	0.41
1:F:290:LEU:HG	2:N:66:LEU:HD11	2.01	0.41
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.56	0.41
1:E:150:GLY:HA3	1:E:371[B]:MET:SD	2.60	0.41
1:E:277:ASN:HD21	1:E:293:ILE:HD12	1.85	0.41
1:F:48:VAL:CG1	1:F:53[B]:CYS:SG	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1174:HOH:O	2:L:10:LYS:HE3	2.21	0.41
1:A:177:LYS:HG2	1:A:203:ASP:OD2	2.21	0.41
1:B:90:VAL:HA	1:B:91:PRO:HD2	1.63	0.41
1:B:175:LYS:HA	1:B:176:PRO:C	2.40	0.41
1:C:241:ASN:HA	1:C:266:MET:HG3	2.03	0.41
1:C:259[B]:GLU:OE1	2:I:61:GLY:HA3	2.21	0.41
1:A:21:ARG:NH1	6:A:1016:HOH:O	2.54	0.41
2:N:113:GLN:NE2	6:N:1088:HOH:O	2.53	0.41
1:B:371[B]:MET:SD	6:B:1127:HOH:O	2.63	0.41
1:E:153:HIS:HE1	6:E:1209:HOH:O	2.03	0.41
1:E:170:LEU:HG	1:E:424:LEU:HD22	2.02	0.41
2:N:128:THR:HG23	6:N:1102:HOH:O	2.20	0.41
1:D:201:KCX:HB2	1:D:239:TYR:CD2	2.57	0.40
1:F:190:TYR:CZ	1:F:227:LYS:HE3	2.56	0.40
2:J:39:ILE:O	2:J:109:ALA:HA	2.20	0.40
2:P:32[A]:TYR:CE2	2:P:38:TRP:HZ3	2.39	0.40
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.55	0.40
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.56	0.40
1:F:190:TYR:CZ	1:F:194:ARG:HD3	2.56	0.40
1:D:175:LYS:HA	1:D:176:PRO:C	2.42	0.40
1:G:449:CYS:O	1:G:456:ALA:HB2	2.21	0.40
2:I:107:LEU:O	2:I:120:GLY:HA2	2.20	0.40
2:J:85:ASP:HA	2:J:86:PRO:HD2	1.95	0.40
1:A:48:VAL:HG12	1:A:53[B]:CYS:SG	2.61	0.40
1:A:298:HIS:ND1	1:A:302:ASP:OD2	2.35	0.40
1:B:449:CYS:HB3	1:B:456:ALA:HA	2.03	0.40
1:F:170:LEU:HD11	1:F:421:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/475 (99%)	456 (97%)	13 (3%)	0	100	100
1	B	469/475 (99%)	454 (97%)	14 (3%)	1 (0%)	47	23
1	C	468/475 (98%)	454 (97%)	14 (3%)	0	100	100
1	D	469/475 (99%)	456 (97%)	13 (3%)	0	100	100
1	E	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	F	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	G	467/475 (98%)	453 (97%)	14 (3%)	0	100	100
1	H	471/475 (99%)	458 (97%)	12 (2%)	1 (0%)	47	23
2	I	141/140 (101%)	136 (96%)	5 (4%)	0	100	100
2	J	142/140 (101%)	138 (97%)	4 (3%)	0	100	100
2	K	143/140 (102%)	138 (96%)	5 (4%)	0	100	100
2	L	144/140 (103%)	139 (96%)	5 (4%)	0	100	100
2	M	144/140 (103%)	137 (95%)	7 (5%)	0	100	100
2	N	143/140 (102%)	138 (96%)	5 (4%)	0	100	100
2	O	144/140 (103%)	139 (96%)	5 (4%)	0	100	100
2	P	143/140 (102%)	137 (96%)	6 (4%)	0	100	100
All	All	4891/4920 (99%)	4741 (97%)	148 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	PRO
1	H	337	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	377/376 (100%)	372 (99%)	5 (1%)	69	44
1	B	377/376 (100%)	370 (98%)	7 (2%)	57	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	376/376 (100%)	372 (99%)	4 (1%)	73	53
1	D	378/376 (100%)	374 (99%)	4 (1%)	73	53
1	E	377/376 (100%)	373 (99%)	4 (1%)	73	53
1	F	377/376 (100%)	373 (99%)	4 (1%)	73	53
1	G	377/376 (100%)	371 (98%)	6 (2%)	62	36
1	H	379/376 (101%)	373 (98%)	6 (2%)	62	36
2	I	125/122 (102%)	122 (98%)	3 (2%)	49	19
2	J	126/122 (103%)	123 (98%)	3 (2%)	49	19
2	K	127/122 (104%)	125 (98%)	2 (2%)	62	36
2	L	128/122 (105%)	126 (98%)	2 (2%)	62	36
2	M	128/122 (105%)	125 (98%)	3 (2%)	50	20
2	N	127/122 (104%)	125 (98%)	2 (2%)	62	36
2	O	128/122 (105%)	126 (98%)	2 (2%)	62	36
2	P	127/122 (104%)	125 (98%)	2 (2%)	62	36
All	All	4034/3984 (101%)	3975 (98%)	59 (2%)	65	39

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	TYR
1	A	203	ASP
1	A	239	TYR
1	A	241	ASN
1	A	392	GLU
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	392	GLU
1	B	439	ARG
1	B	460	GLU
1	B	464	GLU
1	C	203	ASP
1	C	239	TYR
1	C	241	ASN
1	C	392	GLU
1	D	185	TYR
1	D	203	ASP

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Mol	Chain	Res	Type
1	D	241	ASN
1	D	392	GLU
1	E	185	TYR
1	E	203	ASP
1	E	239	TYR
1	E	241	ASN
1	F	185	TYR
1	F	203	ASP
1	F	239	TYR
1	F	241	ASN
1	G	94[A]	ASP
1	G	94[B]	ASP
1	G	203	ASP
1	G	239	TYR
1	G	241	ASN
1	G	445	ILE
1	H	163	ASN
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	392	GLU
2	I	9	ASN
2	I	12	PHE
2	I	137	LYS
2	J	9	ASN
2	J	12	PHE
2	J	98	LYS
2	K	9	ASN
2	K	12	PHE
2	L	9	ASN
2	L	12	PHE
2	M	9	ASN
2	M	12	PHE
2	M	125	ARG
2	N	9	ASN
2	N	12	PHE
2	O	9	ASN
2	O	88	GLN
2	P	9	ASN
2	P	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	432	ASN
1	C	153	HIS
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	386	HIS
1	C	401	GLN
1	C	432	ASN
1	D	153	HIS
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	267	HIS
1	D	277	ASN
1	D	304	GLN
1	D	386	HIS
1	D	401	GLN
1	D	420	ASN
1	D	432	ASN
1	E	153	HIS

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Mol	Chain	Res	Type
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	432	ASN
1	F	153	HIS
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	304	GLN
1	F	386	HIS
1	F	401	GLN
1	F	432	ASN
1	G	153	HIS
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	386	HIS
1	G	401	GLN
1	G	432	ASN
1	H	153	HIS
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	432	ASN
2	I	8	ASN
2	I	9	ASN
2	I	25	GLN

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Mol	Chain	Res	Type
2	I	29	GLN
2	I	115	GLN
2	I	133	GLN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	113	GLN
2	J	115	GLN
2	J	133	GLN
2	K	9	ASN
2	K	25	GLN
2	K	29	GLN
2	K	115	GLN
2	K	133	GLN
2	L	9	ASN
2	L	25	GLN
2	L	29	GLN
2	L	115	GLN
2	M	8	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	113	GLN
2	M	115	GLN
2	M	133	GLN
2	N	8	ASN
2	N	9	ASN
2	N	25	GLN
2	N	29	GLN
2	N	113	GLN
2	N	115	GLN
2	N	133	GLN
2	O	8	ASN
2	O	9	ASN
2	O	25	GLN
2	O	29	GLN
2	O	115	GLN
2	O	133	GLN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	115	GLN

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Mol	Chain	Res	Type
2	P	133	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 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	KCX	G	201	1,3	7,11,12	0.79	0	4,12,14	0.51	0
2	MME	J	1	2	7,8,9	2.86	1 (14%)	5,8,10	1.29	1 (20%)
2	MME	N	1	2	7,8,9	2.85	1 (14%)	5,8,10	1.38	0
1	HYP	G	151	1	6,8,9	0.58	0	5,10,12	1.25	1 (20%)
1	HYP	E	151	1	6,8,9	0.63	0	5,10,12	1.71	1 (20%)
1	SMC	C	256	1	5,6,7	0.98	0	2,6,8	0.63	0
1	KCX	F	201	1,3	7,11,12	0.91	0	4,12,14	0.29	0
1	SMC	H	369	1	5,6,7	0.63	0	2,6,8	0.86	0
1	SMC	D	256	1	5,6,7	0.55	0	2,6,8	0.89	0
1	SMC	G	369	1	5,6,7	0.68	0	2,6,8	1.21	0
1	KCX	E	201	1,3	7,11,12	0.78	0	4,12,14	0.25	0
1	HYP	A	151	1	6,8,9	0.59	0	5,10,12	1.37	0
2	MME	O	1	2	7,8,9	2.84	1 (14%)	5,8,10	1.19	0
1	SMC	E	369	1	5,6,7	0.77	0	2,6,8	0.68	0
1	HYP	D	104	1	6,8,9	0.63	0	5,10,12	0.90	0
1	SMC	A	369	1	5,6,7	0.59	0	2,6,8	1.37	0
1	HYP	D	151	1	6,8,9	0.71	0	5,10,12	1.25	0
1	SMC	H	256	1	5,6,7	0.67	0	2,6,8	0.14	0
1	KCX	H	201	1,3	7,11,12	0.71	0	4,12,14	0.57	0
1	HYP	F	151	1	6,8,9	0.55	0	5,10,12	1.39	1 (20%)
1	KCX	B	201	1,3	7,11,12	0.70	0	4,12,14	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SMC	C	369	1	5,6,7	0.89	0	2,6,8	1.24	0
1	HYP	C	151	1	6,8,9	0.64	0	5,10,12	1.37	0
1	SMC	B	256	1	5,6,7	0.91	0	2,6,8	0.84	0
1	KCX	A	201	1,3	7,11,12	0.89	0	4,12,14	0.21	0
2	MME	M	1	2	7,8,9	2.82	1 (14%)	5,8,10	1.36	1 (20%)
1	HYP	E	104	1	6,8,9	0.54	0	5,10,12	0.89	0
1	HYP	G	104	1	6,8,9	0.44	0	5,10,12	0.89	0
1	HYP	F	104	1	6,8,9	0.53	0	5,10,12	1.00	0
1	KCX	D	201	1,3	7,11,12	0.76	0	4,12,14	0.33	0
1	HYP	C	104	1	6,8,9	0.35	0	5,10,12	0.90	0
1	HYP	B	151	1	6,8,9	0.48	0	5,10,12	1.64	2 (40%)
1	SMC	B	369	1	5,6,7	0.92	0	2,6,8	1.81	1 (50%)
1	SMC	G	256	1	5,6,7	0.67	0	2,6,8	0.41	0
2	MME	L	1	2	7,8,9	2.88	1 (14%)	5,8,10	1.34	1 (20%)
2	MME	K	1	2	7,8,9	2.90	1 (14%)	5,8,10	1.20	0
1	HYP	H	104	1	6,8,9	0.60	0	5,10,12	0.97	0
1	KCX	C	201	1,3	7,11,12	1.07	0	4,12,14	0.34	0
1	SMC	F	256	1	5,6,7	0.73	0	2,6,8	0.95	0
1	HYP	H	151	1	6,8,9	0.58	0	5,10,12	1.32	0
1	SMC	F	369	1	5,6,7	0.76	0	2,6,8	1.57	0
2	MME	P	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.25	0
1	HYP	A	104	1	6,8,9	0.61	0	5,10,12	0.94	0
1	HYP	B	104	1	6,8,9	0.60	0	5,10,12	0.94	0
2	MME	I	1	2	7,8,9	2.86	1 (14%)	5,8,10	1.16	0
1	SMC	A	256	1	5,6,7	0.69	0	2,6,8	0.60	0
1	SMC	D	369	1	5,6,7	0.79	0	2,6,8	1.58	0
1	SMC	E	256	1	5,6,7	0.77	0	2,6,8	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	201	1,3	-	0/7/10/12	-
2	MME	J	1	2	-	0/5/8/10	-
2	MME	N	1	2	-	1/5/8/10	-
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	SMC	C	256	1	-	0/3/5/7	-
1	KCX	F	201	1,3	-	0/7/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	H	369	1	-	1/3/5/7	-
1	SMC	D	256	1	-	0/3/5/7	-
1	SMC	G	369	1	-	1/3/5/7	-
1	KCX	E	201	1,3	-	0/7/10/12	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
2	MME	O	1	2	-	3/5/8/10	-
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	SMC	A	369	1	-	1/3/5/7	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	SMC	H	256	1	-	0/3/5/7	-
1	KCX	H	201	1,3	-	0/7/10/12	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/7/10/12	-
1	SMC	C	369	1	-	1/3/5/7	-
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	SMC	B	256	1	-	0/3/5/7	-
1	KCX	A	201	1,3	-	0/7/10/12	-
2	MME	M	1	2	-	3/5/8/10	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	KCX	D	201	1,3	-	0/7/10/12	-
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	SMC	B	369	1	-	1/3/5/7	-
1	SMC	G	256	1	-	0/3/5/7	-
2	MME	L	1	2	-	1/5/8/10	-
2	MME	K	1	2	-	2/5/8/10	-
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	KCX	C	201	1,3	-	0/7/10/12	-
1	SMC	F	256	1	-	0/3/5/7	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	SMC	F	369	1	-	1/3/5/7	-
2	MME	P	1	2	-	2/5/8/10	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
2	MME	I	1	2	-	1/5/8/10	-
1	SMC	A	256	1	-	0/3/5/7	-
1	SMC	D	369	1	-	1/3/5/7	-
1	SMC	E	256	1	-	0/3/5/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	MME	CM-N	-7.40	1.27	1.46
2	P	1	MME	CM-N	-7.36	1.27	1.46
2	L	1	MME	CM-N	-7.36	1.27	1.46
2	J	1	MME	CM-N	-7.29	1.27	1.46
2	O	1	MME	CM-N	-7.28	1.27	1.46
2	I	1	MME	CM-N	-7.26	1.27	1.46
2	N	1	MME	CM-N	-7.21	1.27	1.46
2	M	1	MME	CM-N	-7.18	1.27	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	HYP	CB-CG-CD	-3.18	99.36	103.27
1	B	369	SMC	CA-CB-SG	-2.43	110.12	114.04
2	J	1	MME	CM-N-CA	2.16	120.37	113.64
2	M	1	MME	CM-N-CA	2.13	120.25	113.64
1	B	151	HYP	O-C-CA	-2.11	119.24	124.78
1	F	151	HYP	O-C-CA	-2.08	119.34	124.78
2	L	1	MME	CM-N-CA	2.06	120.05	113.64
1	G	151	HYP	O-C-CA	-2.04	119.44	124.78
1	B	151	HYP	OD1-CG-CD	-2.00	105.97	110.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	MME	C-CA-CB-CG
2	L	1	MME	CB-CG-SD-CE
2	K	1	MME	CB-CG-SD-CE
2	I	1	MME	CB-CG-SD-CE
2	O	1	MME	N-CA-CB-CG
2	M	1	MME	C-CA-CB-CG
2	P	1	MME	C-CA-CB-CG
2	M	1	MME	CB-CG-SD-CE
2	P	1	MME	CB-CG-SD-CE
1	H	369	SMC	N-CA-CB-SG
1	G	369	SMC	N-CA-CB-SG
1	E	369	SMC	N-CA-CB-SG
1	A	369	SMC	N-CA-CB-SG
1	C	369	SMC	N-CA-CB-SG
1	B	369	SMC	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	F	369	SMC	N-CA-CB-SG
1	D	369	SMC	N-CA-CB-SG
2	N	1	MME	C-CA-CB-CG
2	K	1	MME	C-CA-CB-CG
2	O	1	MME	CB-CG-SD-CE
2	M	1	MME	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	201	KCX	1	0
1	H	201	KCX	1	0
1	D	201	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	H	1479	-	3,3,3	0.68	0	2,2,2	0.12	0
5	EDO	F	1481	-	3,3,3	0.56	0	2,2,2	0.28	0
4	CAP	B	1477	3	15,20,20	0.86	0	20,31,31	0.75	0
5	EDO	B	1481	-	3,3,3	0.51	0	2,2,2	0.28	0
5	EDO	D	1481	-	3,3,3	0.52	0	2,2,2	0.19	0
5	EDO	A	1483	-	3,3,3	0.55	0	2,2,2	0.07	0
5	EDO	H	1478	-	3,3,3	0.46	0	2,2,2	0.10	0
5	EDO	E	1478	-	3,3,3	0.69	0	2,2,2	0.11	0
5	EDO	A	1482	-	3,3,3	0.49	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	1478	-	3,3,3	0.51	0	2,2,2	0.18	0
5	EDO	C	1482	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	L	1141	-	3,3,3	0.53	0	2,2,2	0.14	0
5	EDO	M	1141	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	B	1480	-	3,3,3	0.55	0	2,2,2	0.31	0
5	EDO	G	1480	-	3,3,3	0.59	0	2,2,2	0.17	0
5	EDO	J	1141	-	3,3,3	0.50	0	2,2,2	0.19	0
4	CAP	D	1477	3	15,20,20	0.96	0	20,31,31	0.68	0
4	CAP	G	1477	3	15,20,20	1.08	1 (6%)	20,31,31	0.63	0
4	CAP	F	1477	3	15,20,20	0.74	0	20,31,31	0.65	0
5	EDO	E	1480	-	3,3,3	0.62	0	2,2,2	0.12	0
5	EDO	I	1142	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	C	1483	-	3,3,3	0.50	0	2,2,2	0.11	0
5	EDO	L	1142	-	3,3,3	0.47	0	2,2,2	0.41	0
5	EDO	D	1482	-	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	N	1142	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	G	1479	-	3,3,3	0.57	0	2,2,2	0.16	0
5	EDO	C	1478	-	3,3,3	0.68	0	2,2,2	0.14	0
5	EDO	D	1480	-	3,3,3	0.52	0	2,2,2	0.31	0
5	EDO	O	1141	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	P	1142	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	N	1141	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	F	1480	-	3,3,3	0.51	0	2,2,2	0.06	0
5	EDO	C	1481	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	I	1141	-	3,3,3	0.51	0	2,2,2	0.24	0
5	EDO	M	1142	-	3,3,3	0.44	0	2,2,2	0.52	0
5	EDO	A	1484	-	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	K	1142	-	3,3,3	0.46	0	2,2,2	0.35	0
4	CAP	C	1477	3	15,20,20	0.97	0	20,31,31	0.66	0
4	CAP	E	1477	3	15,20,20	0.92	1 (6%)	20,31,31	0.68	0
5	EDO	K	1141	-	3,3,3	0.50	0	2,2,2	0.23	0
5	EDO	B	1479	-	3,3,3	0.49	0	2,2,2	0.15	0
5	EDO	B	1478	-	3,3,3	0.50	0	2,2,2	0.32	0
5	EDO	G	1478	-	3,3,3	0.66	0	2,2,2	0.19	0
5	EDO	G	1482	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	B	1482	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	F	1482	-	3,3,3	0.42	0	2,2,2	0.46	0
5	EDO	E	1481	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	E	1479	-	3,3,3	0.56	0	2,2,2	0.17	0
5	EDO	G	1481	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	C	1480	-	3,3,3	0.52	0	2,2,2	0.30	0
5	EDO	A	1479	-	3,3,3	0.40	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	1480	-	3,3,3	0.52	0	2,2,2	0.29	0
5	EDO	D	1479	-	3,3,3	0.45	0	2,2,2	0.16	0
5	EDO	F	1479	-	3,3,3	0.61	0	2,2,2	0.12	0
5	EDO	H	1480	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	F	1478	-	3,3,3	0.54	0	2,2,2	0.16	0
5	EDO	D	1478	-	3,3,3	0.61	0	2,2,2	0.25	0
5	EDO	P	1141	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	J	1142	-	3,3,3	0.42	0	2,2,2	0.50	0
5	EDO	C	1479	-	3,3,3	0.51	0	2,2,2	0.14	0
4	CAP	A	1477	3	15,20,20	0.97	1 (6%)	20,31,31	0.60	0
5	EDO	A	1481	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	F	1483	-	3,3,3	0.45	0	2,2,2	0.28	0
5	EDO	H	1482	-	3,3,3	0.55	0	2,2,2	0.21	0
4	CAP	H	1477	3	15,20,20	1.05	0	20,31,31	0.95	1 (5%)
5	EDO	O	1142	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	H	1481	-	3,3,3	0.52	0	2,2,2	0.27	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
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	F	1481	-	-	0/1/1/1	-
4	CAP	B	1477	3	-	3/23/29/29	-
5	EDO	B	1481	-	-	0/1/1/1	-
5	EDO	D	1481	-	-	0/1/1/1	-
5	EDO	A	1483	-	-	0/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
5	EDO	A	1482	-	-	1/1/1/1	-
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	C	1482	-	-	1/1/1/1	-
5	EDO	L	1141	-	-	0/1/1/1	-
5	EDO	M	1141	-	-	0/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	G	1480	-	-	0/1/1/1	-
5	EDO	J	1141	-	-	0/1/1/1	-
4	CAP	D	1477	3	-	2/23/29/29	-
4	CAP	G	1477	3	-	2/23/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	F	1477	3	-	2/23/29/29	-
5	EDO	E	1480	-	-	0/1/1/1	-
5	EDO	I	1142	-	-	0/1/1/1	-
5	EDO	C	1483	-	-	0/1/1/1	-
5	EDO	L	1142	-	-	0/1/1/1	-
5	EDO	D	1482	-	-	1/1/1/1	-
5	EDO	N	1142	-	-	0/1/1/1	-
5	EDO	G	1479	-	-	1/1/1/1	-
5	EDO	C	1478	-	-	0/1/1/1	-
5	EDO	D	1480	-	-	0/1/1/1	-
5	EDO	O	1141	-	-	0/1/1/1	-
5	EDO	P	1142	-	-	0/1/1/1	-
5	EDO	N	1141	-	-	0/1/1/1	-
5	EDO	F	1480	-	-	1/1/1/1	-
5	EDO	C	1481	-	-	0/1/1/1	-
5	EDO	I	1141	-	-	0/1/1/1	-
5	EDO	M	1142	-	-	0/1/1/1	-
5	EDO	A	1484	-	-	0/1/1/1	-
5	EDO	K	1142	-	-	0/1/1/1	-
4	CAP	C	1477	3	-	3/23/29/29	-
4	CAP	E	1477	3	-	3/23/29/29	-
5	EDO	K	1141	-	-	0/1/1/1	-
5	EDO	B	1479	-	-	1/1/1/1	-
5	EDO	B	1478	-	-	0/1/1/1	-
5	EDO	G	1478	-	-	0/1/1/1	-
5	EDO	G	1482	-	-	1/1/1/1	-
5	EDO	B	1482	-	-	1/1/1/1	-
5	EDO	F	1482	-	-	0/1/1/1	-
5	EDO	E	1481	-	-	0/1/1/1	-
5	EDO	E	1479	-	-	0/1/1/1	-
5	EDO	G	1481	-	-	0/1/1/1	-
5	EDO	C	1480	-	-	0/1/1/1	-
5	EDO	A	1479	-	-	1/1/1/1	-
5	EDO	A	1480	-	-	0/1/1/1	-
5	EDO	D	1479	-	-	1/1/1/1	-
5	EDO	F	1479	-	-	0/1/1/1	-
5	EDO	H	1480	-	-	1/1/1/1	-
5	EDO	F	1478	-	-	0/1/1/1	-
5	EDO	D	1478	-	-	0/1/1/1	-
5	EDO	P	1141	-	-	0/1/1/1	-
5	EDO	J	1142	-	-	1/1/1/1	-
5	EDO	C	1479	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	A	1477	3	-	2/23/29/29	-
5	EDO	A	1481	-	-	0/1/1/1	-
5	EDO	F	1483	-	-	1/1/1/1	-
5	EDO	H	1482	-	-	0/1/1/1	-
4	CAP	H	1477	3	-	3/23/29/29	-
5	EDO	O	1142	-	-	0/1/1/1	-
5	EDO	H	1481	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1477	CAP	O2-C2	2.26	1.46	1.43
4	E	1477	CAP	O2-C2	2.05	1.46	1.43
4	A	1477	CAP	O2-C2	2.00	1.46	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1477	CAP	O4-C4-C5	-2.44	104.44	109.92

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1477	CAP	O3-C3-C4-O4
4	D	1477	CAP	O3-C3-C4-O4
4	G	1477	CAP	O3-C3-C4-O4
4	F	1477	CAP	O3-C3-C4-O4
4	C	1477	CAP	O3-C3-C4-O4
4	E	1477	CAP	O3-C3-C4-O4
4	A	1477	CAP	O3-C3-C4-O4
4	H	1477	CAP	C2-C3-C4-O4
4	H	1477	CAP	O3-C3-C4-O4
5	A	1482	EDO	O1-C1-C2-O2
5	G	1479	EDO	O1-C1-C2-O2
5	G	1482	EDO	O1-C1-C2-O2
5	A	1479	EDO	O1-C1-C2-O2
5	H	1480	EDO	O1-C1-C2-O2
4	B	1477	CAP	O2-C2-C3-C4
4	D	1477	CAP	O2-C2-C3-C4
4	G	1477	CAP	O2-C2-C3-C4

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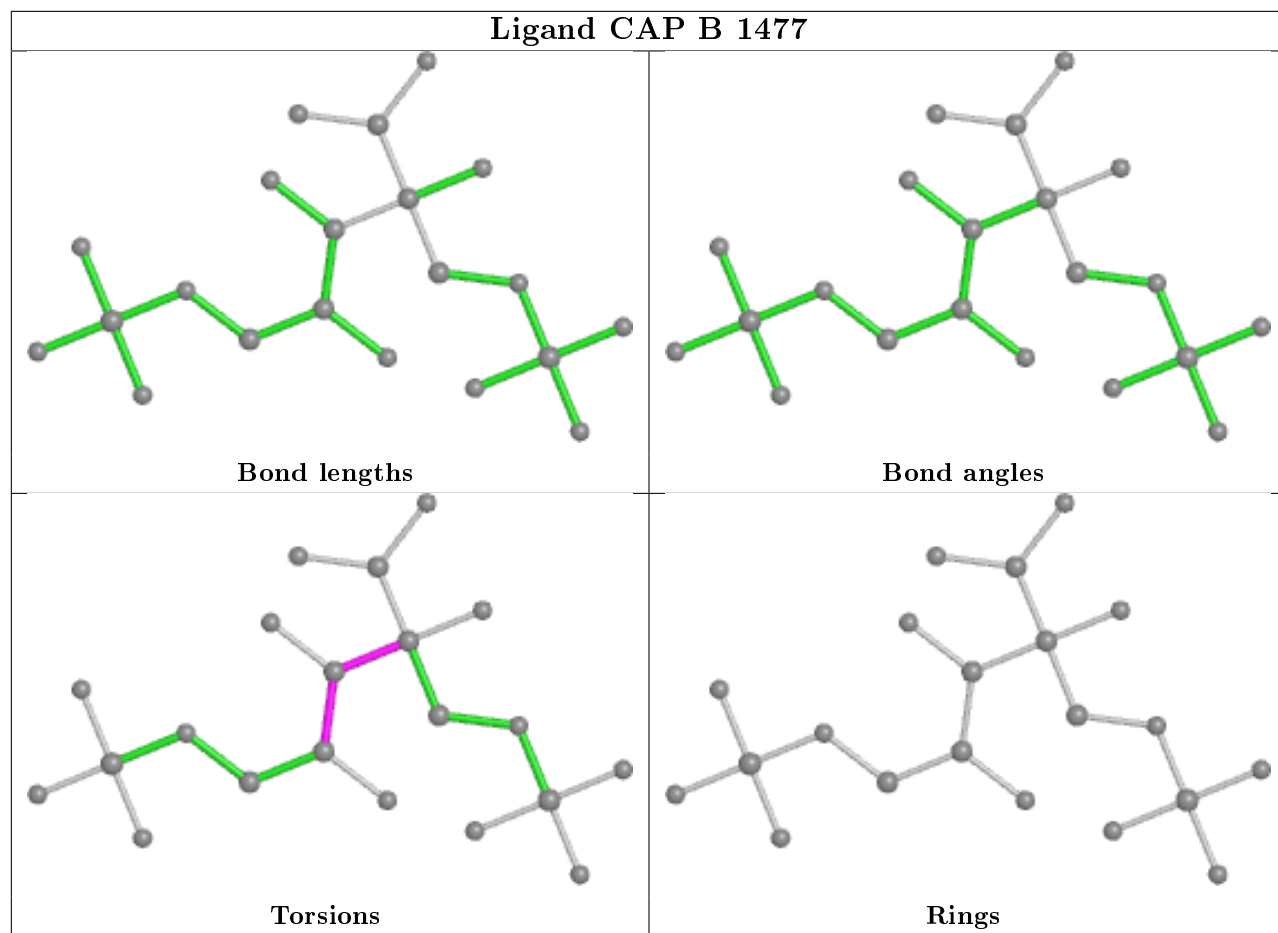
Mol	Chain	Res	Type	Atoms
4	F	1477	CAP	O2-C2-C3-C4
4	C	1477	CAP	O2-C2-C3-C4
4	E	1477	CAP	O2-C2-C3-C4
4	A	1477	CAP	O2-C2-C3-C4
4	H	1477	CAP	O2-C2-C3-C4
5	D	1479	EDO	O1-C1-C2-O2
5	C	1482	EDO	O1-C1-C2-O2
5	B	1479	EDO	O1-C1-C2-O2
5	C	1479	EDO	O1-C1-C2-O2
5	F	1483	EDO	O1-C1-C2-O2
5	D	1482	EDO	O1-C1-C2-O2
4	B	1477	CAP	C2-C3-C4-O4
4	C	1477	CAP	C2-C3-C4-O4
5	F	1480	EDO	O1-C1-C2-O2
4	E	1477	CAP	C2-C3-C4-O4
5	J	1142	EDO	O1-C1-C2-O2
5	B	1482	EDO	O1-C1-C2-O2

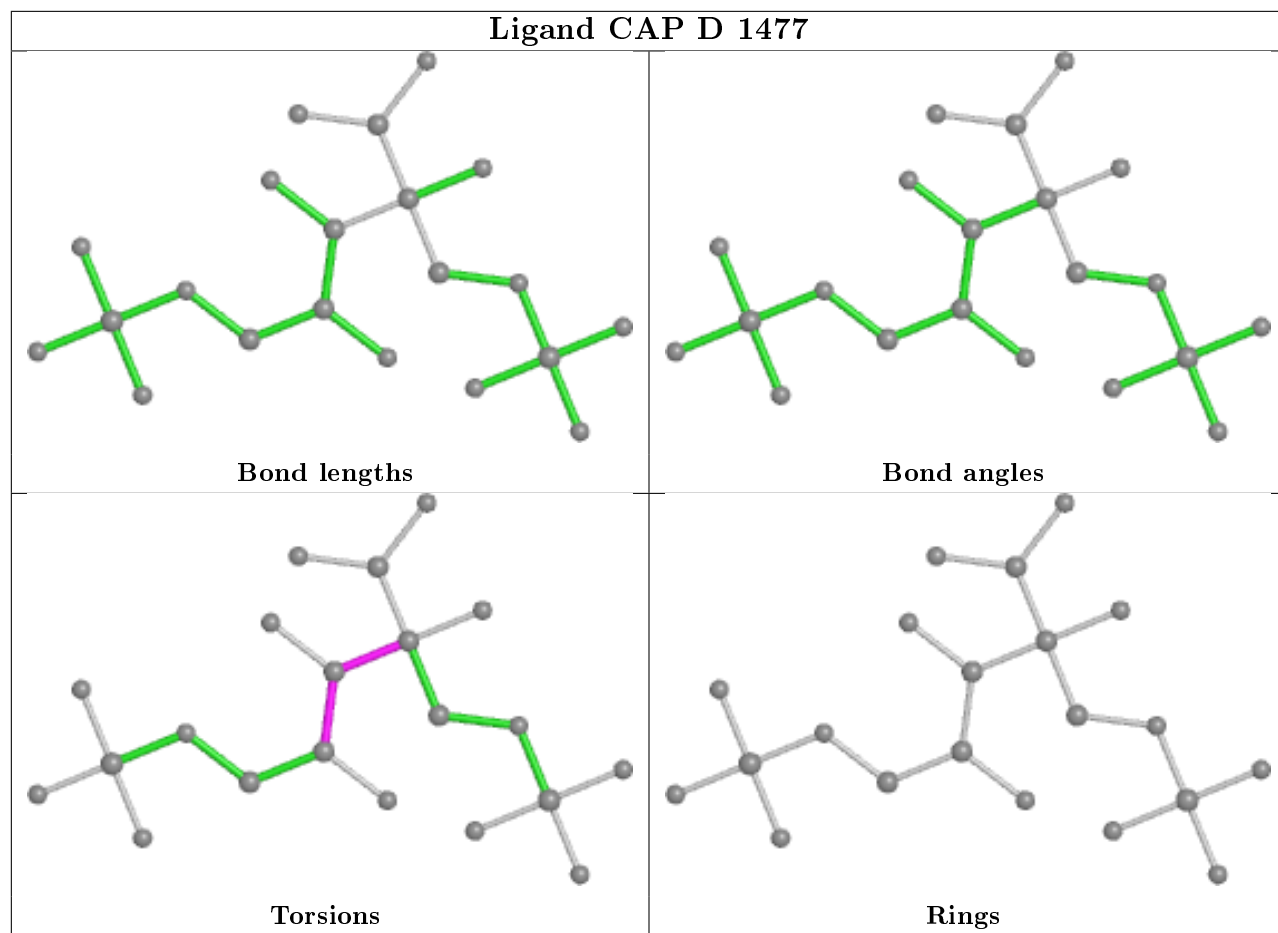
There are no ring outliers.

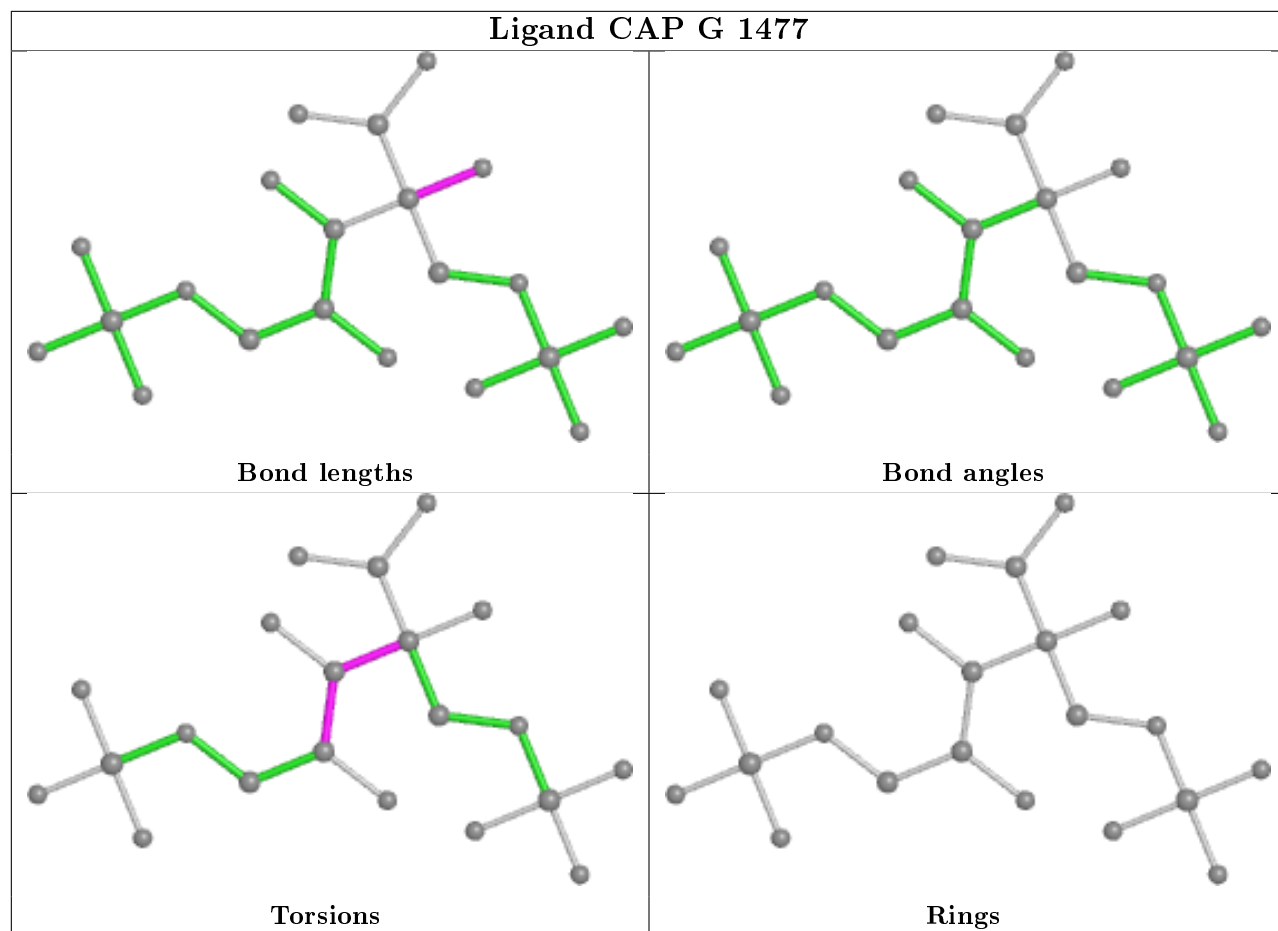
2 monomers are involved in 2 short contacts:

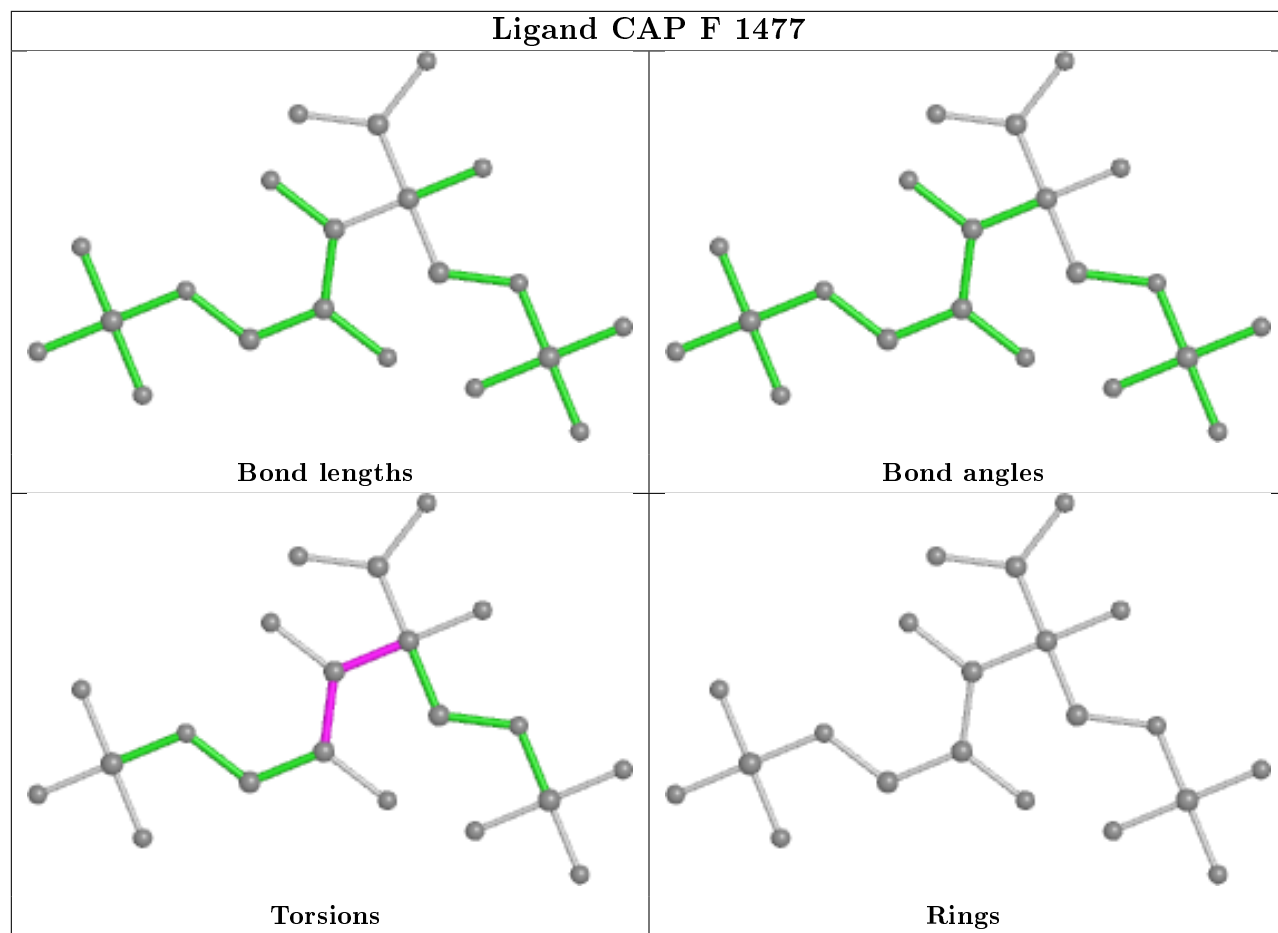
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1482	EDO	1	0
5	F	1483	EDO	1	0

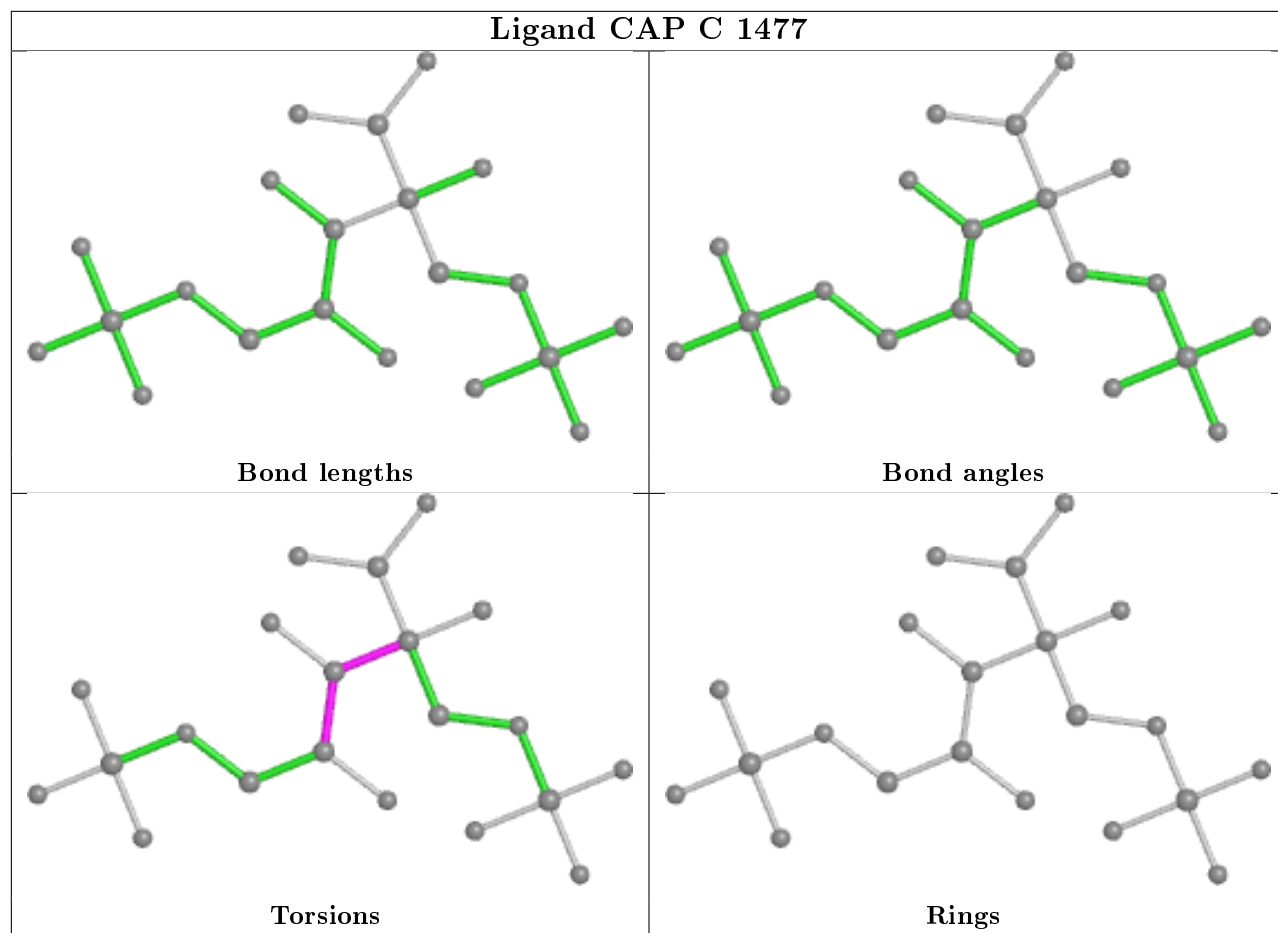
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



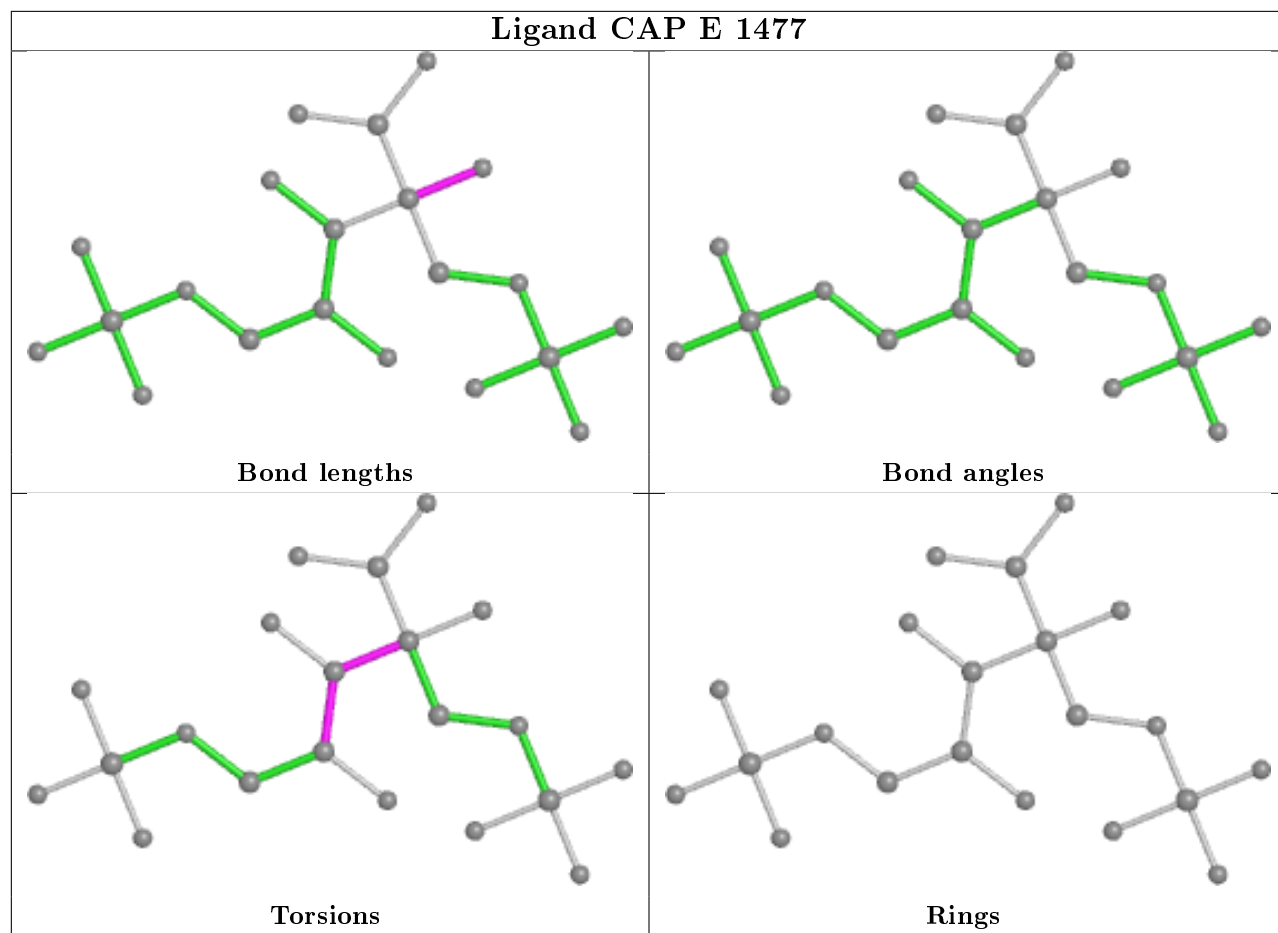


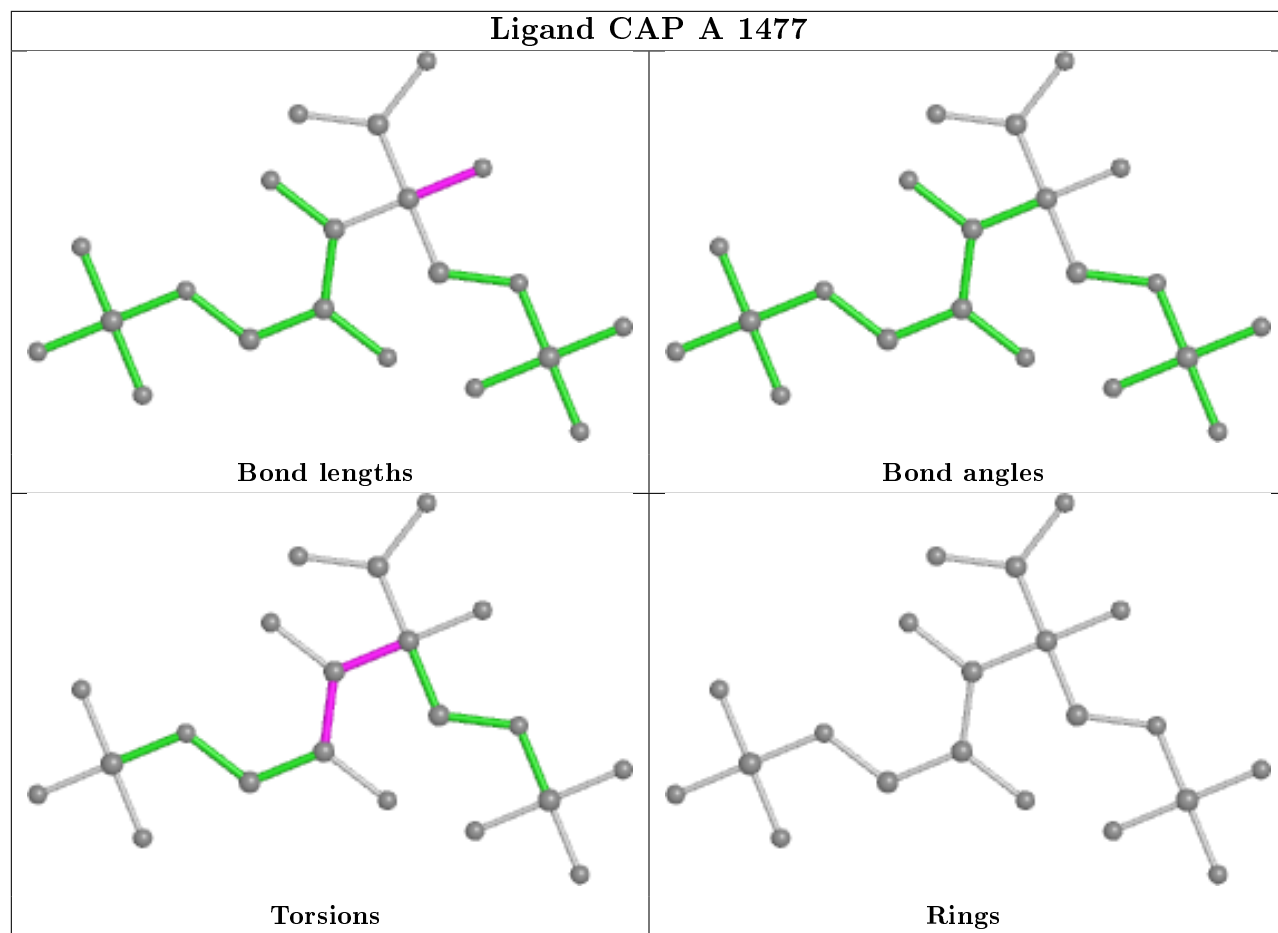


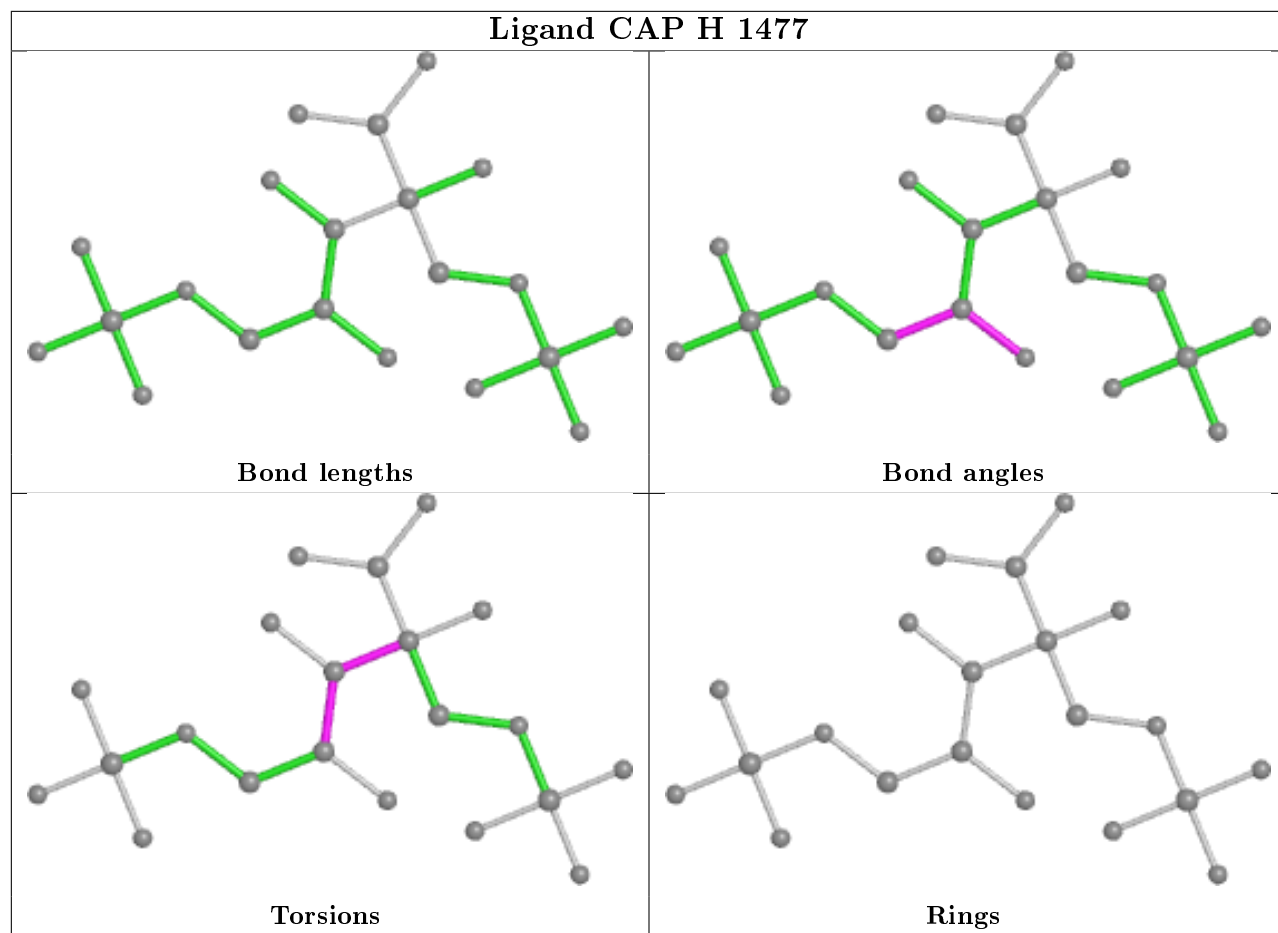












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	462/475 (97%)	-0.10	14 (3%)	50	55	10, 15, 28, 40	0
1	B	462/475 (97%)	-0.09	17 (3%)	41	46	10, 15, 28, 40	0
1	C	462/475 (97%)	-0.12	20 (4%)	35	39	10, 16, 28, 41	0
1	D	461/475 (97%)	-0.11	14 (3%)	50	55	11, 16, 27, 40	0
1	E	460/475 (96%)	-0.17	10 (2%)	62	67	10, 15, 28, 41	0
1	F	460/475 (96%)	-0.16	14 (3%)	50	55	11, 16, 28, 39	0
1	G	460/475 (96%)	-0.10	14 (3%)	50	55	10, 15, 28, 41	0
1	H	462/475 (97%)	-0.06	18 (3%)	39	44	10, 16, 28, 40	0
2	I	139/140 (99%)	0.35	15 (10%)	5	5	14, 21, 32, 36	0
2	J	139/140 (99%)	0.26	12 (8%)	10	11	14, 20, 33, 36	0
2	K	139/140 (99%)	0.31	14 (10%)	7	7	14, 21, 33, 37	0
2	L	139/140 (99%)	0.18	10 (7%)	15	16	14, 21, 32, 35	0
2	M	139/140 (99%)	0.17	9 (6%)	18	20	13, 20, 33, 35	0
2	N	139/140 (99%)	0.25	11 (7%)	12	13	14, 21, 33, 36	0
2	O	139/140 (99%)	0.19	12 (8%)	10	11	14, 20, 33, 36	0
2	P	139/140 (99%)	0.55	18 (12%)	3	3	14, 21, 33, 37	0
All	All	4801/4920 (97%)	-0.02	222 (4%)	32	35	10, 17, 30, 41	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	475	LEU	10.7
1	D	10	GLY	9.3
2	P	136	ASN	9.0
1	H	9	ALA	8.7
1	D	475	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	475	LEU	7.9
1	A	9	ALA	7.8
1	E	475	LEU	7.8
1	G	475	LEU	7.4
1	G	94[A]	ASP	7.3
1	B	10	GLY	7.2
2	P	140	VAL	7.1
1	C	11	ALA	6.8
1	A	10	GLY	6.8
1	H	11	ALA	6.7
1	F	475	LEU	6.6
1	H	475	LEU	6.5
1	F	11	ALA	6.5
1	C	9	ALA	6.4
1	D	11	ALA	6.4
1	H	94[A]	ASP	6.3
2	P	135	ALA	6.2
1	C	10	GLY	6.2
1	G	92	GLY	6.1
1	E	94[A]	ASP	5.8
1	B	9	ALA	5.7
1	F	94[A]	ASP	5.7
1	G	11	ALA	5.7
1	H	91	PRO	5.6
1	A	94[A]	ASP	5.6
1	H	10	GLY	5.6
1	E	11	ALA	5.6
1	D	92	GLY	5.5
1	D	94[A]	ASP	5.5
2	P	137	LYS	5.5
1	B	91	PRO	5.5
1	A	475	LEU	5.4
2	P	134	PRO	5.3
1	C	439	ARG	5.2
1	C	92	GLY	5.0
2	K	84	ARG	4.9
1	A	11	ALA	4.8
1	A	439	ARG	4.7
1	B	11	ALA	4.7
2	P	23	ASP	4.6
1	C	94[A]	ASP	4.5
1	G	439	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	94[A]	ASP	4.4
1	D	439	ARG	4.4
1	F	92	GLY	4.4
1	E	439	ARG	4.3
1	H	439	ARG	4.2
1	E	92	GLY	4.2
2	K	136	ASN	4.1
1	C	91	PRO	4.1
1	B	449	CYS	4.0
1	H	438	ALA	3.9
1	C	464	GLU	3.8
2	O	136	ASN	3.8
1	F	464	GLU	3.8
1	F	439	ARG	3.8
2	P	127	LYS	3.7
2	I	130	ARG	3.7
2	P	84	ARG	3.7
1	G	445	ILE	3.6
2	I	140	VAL	3.5
2	N	140	VAL	3.5
1	H	449	CYS	3.5
1	D	449	CYS	3.5
1	G	91	PRO	3.5
2	I	84	ARG	3.5
1	H	451	TRP	3.4
2	N	87	MET	3.4
2	K	128	THR	3.4
2	O	130	ARG	3.4
1	B	464	GLU	3.3
2	I	87	MET	3.3
1	B	359	SER	3.3
2	J	128	THR	3.3
1	G	47	GLY	3.3
1	E	91	PRO	3.3
2	N	128	THR	3.3
2	O	128	THR	3.3
1	D	47	GLY	3.3
1	H	450	LYS	3.3
2	J	136	ASN	3.2
1	A	47	GLY	3.2
2	K	130	ARG	3.2
1	A	464	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	449	CYS	3.2
2	J	127	LYS	3.2
2	N	136	ASN	3.2
1	D	451	TRP	3.2
2	M	130	ARG	3.2
2	I	20	PRO	3.1
2	O	135	ALA	3.1
2	K	87	MET	3.1
2	L	140	VAL	3.1
2	L	127	LYS	3.1
2	J	83	CYS	3.1
2	K	137	LYS	3.1
1	D	464	GLU	3.1
2	K	140	VAL	3.1
2	K	127	LYS	3.1
2	I	88	GLN	3.0
2	P	130	ARG	3.0
1	G	464	GLU	3.0
2	O	84	ARG	3.0
2	I	23	ASP	3.0
1	B	438	ALA	3.0
2	L	128	THR	3.0
2	J	87	MET	3.0
2	P	88	GLN	3.0
1	C	438	ALA	3.0
1	A	451	TRP	2.9
2	P	87	MET	2.9
2	M	136	ASN	2.9
2	P	22	THR	2.9
2	J	140	VAL	2.9
2	P	24	GLU	2.9
1	B	474	LYS	2.9
2	L	136	ASN	2.9
2	J	130	ARG	2.9
1	F	28	ASP	2.8
2	J	84	ARG	2.8
1	C	449	CYS	2.8
2	N	84	ARG	2.8
2	O	127	LYS	2.8
1	H	464	GLU	2.8
1	D	28	ASP	2.8
2	I	127	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	355	GLU	2.8
1	E	464	GLU	2.8
2	J	24	GLU	2.7
1	H	92	GLY	2.7
1	E	93	GLU	2.7
2	N	24	GLU	2.7
2	P	128	THR	2.7
2	L	24	GLU	2.7
1	A	449	CYS	2.7
1	E	47	GLY	2.7
2	O	137	LYS	2.7
1	G	449	CYS	2.7
2	L	87	MET	2.7
2	I	136	ASN	2.6
2	J	137	LYS	2.6
2	M	88	GLN	2.6
1	D	91	PRO	2.6
1	G	93	GLU	2.6
1	A	438	ALA	2.6
2	N	88	GLN	2.6
1	A	443	ASP	2.6
2	N	137	LYS	2.6
1	D	355	GLU	2.6
2	K	135	ALA	2.6
2	K	83	CYS	2.6
2	I	128	THR	2.5
1	C	93	GLU	2.5
1	C	451	TRP	2.5
2	I	24	GLU	2.5
2	O	87[A]	MET	2.4
2	K	24	GLU	2.4
2	N	130	ARG	2.4
2	L	88	GLN	2.4
2	M	84	ARG	2.4
1	C	127	PHE	2.4
1	F	91	PRO	2.4
1	H	460	GLU	2.4
2	P	20	PRO	2.4
2	I	32	TYR	2.4
1	B	450	LYS	2.4
1	H	47	GLY	2.4
2	L	48	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	M	24	GLU	2.4
1	B	470	ASP	2.3
2	M	137	LYS	2.3
1	F	438	ALA	2.3
2	M	23	ASP	2.3
1	A	434	GLY	2.3
2	O	88	GLN	2.3
2	O	140	VAL	2.3
1	D	460	GLU	2.3
2	I	137	LYS	2.3
2	P	83	CYS	2.3
2	L	84	ARG	2.3
2	K	88	GLN	2.3
2	M	127	LYS	2.3
1	C	47	GLY	2.3
1	H	474	LYS	2.2
2	O	24	GLU	2.2
2	P	82	GLY	2.2
1	C	450	LYS	2.2
2	I	48	ASP	2.2
1	F	474	LYS	2.2
2	N	127	LYS	2.2
1	H	443	ASP	2.2
2	O	102	ASP	2.2
1	G	438	ALA	2.2
1	B	460	GLU	2.2
1	C	443	ASP	2.2
2	P	102	ASP	2.2
1	F	93	GLU	2.2
2	N	22	THR	2.1
1	G	443	ASP	2.1
2	J	98	LYS	2.1
2	J	88	GLN	2.1
1	B	28	ASP	2.1
1	C	463	LYS	2.1
1	E	460	GLU	2.1
1	F	443	ASP	2.1
2	K	23	ASP	2.1
1	G	463	LYS	2.1
2	K	22	THR	2.1
2	L	130	ARG	2.1
1	B	468	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	451	TRP	2.1
2	I	22	THR	2.1
2	M	87	MET	2.0
1	B	12	GLY	2.0
1	C	436	ASP	2.0
1	H	12	GLY	2.0
1	A	93	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MME	J	1	9/10	0.85	0.21	27,29,37,38	0
2	MME	N	1	9/10	0.85	0.19	27,28,36,37	0
2	MME	O	1	9/10	0.86	0.20	27,29,37,37	0
2	MME	M	1	9/10	0.86	0.14	26,28,36,36	0
2	MME	I	1	9/10	0.86	0.15	27,28,36,36	0
2	MME	P	1	9/10	0.87	0.17	27,28,35,36	0
2	MME	K	1	9/10	0.89	0.14	27,28,36,37	0
2	MME	L	1	9/10	0.90	0.16	26,28,35,35	0
1	HYP	H	104	8/9	0.96	0.07	13,13,14,15	0
1	HYP	C	151	8/9	0.96	0.06	12,12,13,14	0
1	SMC	A	369	7/8	0.96	0.07	15,16,20,21	0
1	SMC	D	369	7/8	0.96	0.07	15,16,20,22	0
1	KCX	E	201	12/13	0.97	0.07	12,14,15,15	0
1	KCX	A	201	12/13	0.97	0.07	12,13,14,14	0
1	KCX	G	201	12/13	0.97	0.08	12,12,13,13	0
1	HYP	E	104	8/9	0.97	0.06	12,12,13,15	0
1	HYP	G	104	8/9	0.97	0.06	13,13,14,16	0
1	HYP	F	104	8/9	0.97	0.08	13,13,15,16	0
1	HYP	C	104	8/9	0.97	0.06	13,14,14,15	0
1	SMC	B	369	7/8	0.97	0.07	15,16,20,23	0
1	HYP	D	104	8/9	0.97	0.06	13,13,14,16	0
1	KCX	F	201	12/13	0.97	0.07	12,13,14,15	0
1	HYP	D	151	8/9	0.97	0.05	12,12,12,13	0
1	KCX	C	201	12/13	0.97	0.08	13,13,15,15	0
1	SMC	F	369	7/8	0.97	0.07	15,16,20,22	0
1	KCX	H	201	12/13	0.97	0.08	12,12,14,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	B	104	8/9	0.97	0.07	12,13,13,15	0
1	HYP	F	151	8/9	0.97	0.07	12,13,13,13	0
1	SMC	C	369	7/8	0.97	0.07	15,16,20,21	0
1	SMC	E	369	7/8	0.98	0.05	15,15,20,21	0
1	KCX	B	201	12/13	0.98	0.07	12,13,13,15	0
1	SMC	G	369	7/8	0.98	0.05	14,15,19,22	0
1	HYP	H	151	8/9	0.98	0.07	12,12,12,12	0
1	KCX	D	201	12/13	0.98	0.07	12,13,14,15	0
1	HYP	E	151	8/9	0.98	0.06	11,12,12,12	0
1	HYP	A	104	8/9	0.98	0.06	13,13,14,15	0
1	HYP	B	151	8/9	0.98	0.07	12,12,12,13	0
1	HYP	A	151	8/9	0.98	0.07	12,12,12,12	0
1	SMC	H	369	7/8	0.98	0.06	15,16,20,20	0
1	SMC	D	256	7/8	0.99	0.06	11,11,12,13	0
1	SMC	G	256	7/8	0.99	0.05	10,11,12,13	0
1	SMC	B	256	7/8	0.99	0.06	10,11,12,13	0
1	HYP	G	151	8/9	0.99	0.05	12,12,12,13	0
1	SMC	C	256	7/8	0.99	0.06	10,11,13,13	0
1	SMC	H	256	7/8	0.99	0.06	10,11,12,13	0
1	SMC	A	256	7/8	0.99	0.06	11,11,12,14	0
1	SMC	F	256	7/8	0.99	0.05	10,11,12,15	0
1	SMC	E	256	7/8	0.99	0.07	11,11,12,13	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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	G	1480	4/4	0.59	0.22	37,38,38,39	0
5	EDO	F	1481	4/4	0.61	0.16	37,38,38,38	0
5	EDO	N	1142	4/4	0.62	0.23	34,36,37,40	0
5	EDO	A	1480	4/4	0.62	0.17	40,40,41,41	0
5	EDO	B	1480	4/4	0.63	0.15	37,37,37,37	0
5	EDO	D	1480	4/4	0.64	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	I	1142	4/4	0.71	0.19	39,40,41,43	0
5	EDO	A	1484	4/4	0.73	0.23	53,53,54,54	0
5	EDO	C	1482	4/4	0.73	0.20	50,51,51,51	0
5	EDO	E	1480	4/4	0.75	0.17	33,34,34,34	0
5	EDO	B	1482	4/4	0.76	0.25	40,42,43,44	0
5	EDO	C	1480	4/4	0.76	0.16	34,34,35,35	0
5	EDO	A	1482	4/4	0.78	0.23	34,38,38,40	0
5	EDO	M	1142	4/4	0.79	0.15	29,31,32,35	0
5	EDO	G	1482	4/4	0.81	0.14	43,43,43,43	0
5	EDO	H	1481	4/4	0.81	0.13	35,36,36,37	0
5	EDO	D	1482	4/4	0.82	0.15	57,58,58,58	0
5	EDO	H	1482	4/4	0.82	0.20	33,33,34,34	0
5	EDO	G	1479	4/4	0.82	0.13	27,27,28,29	0
5	EDO	O	1141	4/4	0.83	0.15	32,32,33,34	0
5	EDO	J	1142	4/4	0.83	0.17	35,37,38,39	0
5	EDO	L	1141	4/4	0.83	0.17	30,31,31,32	0
5	EDO	O	1142	4/4	0.83	0.15	33,35,36,38	0
5	EDO	J	1141	4/4	0.83	0.15	32,32,33,33	0
5	EDO	I	1141	4/4	0.84	0.17	31,31,33,33	0
5	EDO	L	1142	4/4	0.85	0.15	31,33,35,37	0
5	EDO	N	1141	4/4	0.85	0.13	32,33,33,34	0
5	EDO	M	1141	4/4	0.85	0.21	31,31,32,32	0
5	EDO	K	1141	4/4	0.85	0.17	32,32,34,34	0
5	EDO	F	1483	4/4	0.87	0.21	35,38,38,40	0
5	EDO	P	1141	4/4	0.88	0.11	34,34,35,36	0
5	EDO	P	1142	4/4	0.88	0.16	29,31,33,36	0
5	EDO	B	1481	4/4	0.89	0.13	28,29,29,29	0
5	EDO	A	1479	4/4	0.91	0.10	23,23,23,24	0
5	EDO	D	1478	4/4	0.92	0.11	21,21,22,23	0
5	EDO	K	1142	4/4	0.92	0.15	33,34,35,35	0
5	EDO	E	1478	4/4	0.92	0.12	19,20,22,23	0
5	EDO	F	1479	4/4	0.92	0.09	20,20,22,23	0
5	EDO	C	1478	4/4	0.93	0.11	20,21,22,22	0
5	EDO	B	1478	4/4	0.93	0.12	18,19,20,22	0
5	EDO	G	1478	4/4	0.93	0.10	20,20,22,23	0
5	EDO	H	1479	4/4	0.93	0.10	18,18,20,21	0
5	EDO	A	1481	4/4	0.94	0.10	25,25,25,25	0
5	EDO	G	1481	4/4	0.94	0.15	24,25,26,27	0
5	EDO	E	1479	4/4	0.94	0.09	22,23,23,23	0
5	EDO	B	1479	4/4	0.94	0.09	24,24,25,25	0
5	EDO	C	1483	4/4	0.94	0.06	20,21,22,23	0
5	EDO	F	1482	4/4	0.95	0.13	26,26,26,27	0

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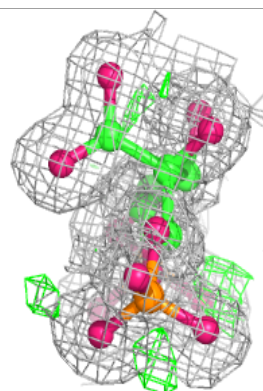
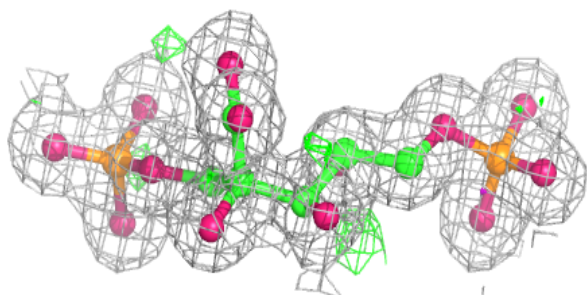
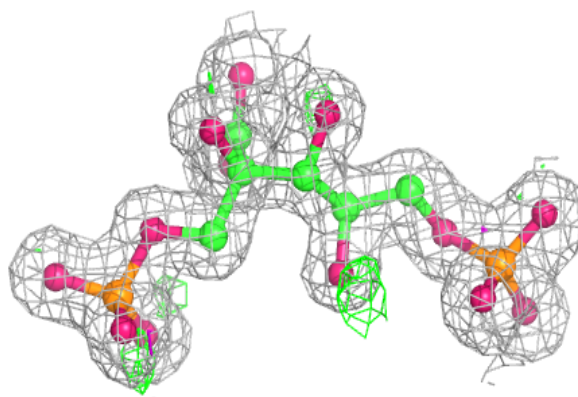
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	1479	4/4	0.95	0.12	24,25,25,28	0
5	EDO	F	1480	4/4	0.95	0.08	25,26,26,26	0
5	EDO	A	1478	4/4	0.95	0.08	18,20,21,21	0
5	EDO	E	1481	4/4	0.96	0.11	25,26,27,28	0
5	EDO	A	1483	4/4	0.96	0.07	19,19,19,20	0
5	EDO	D	1479	4/4	0.96	0.10	25,27,27,27	0
5	EDO	C	1481	4/4	0.96	0.09	30,31,31,31	0
5	EDO	H	1480	4/4	0.96	0.10	25,25,26,27	0
5	EDO	D	1481	4/4	0.97	0.09	25,25,25,26	0
5	EDO	F	1478	4/4	0.97	0.06	19,21,21,21	0
4	CAP	D	1477	21/21	0.98	0.06	13,14,15,19	0
4	CAP	A	1477	21/21	0.98	0.05	13,14,15,19	0
4	CAP	C	1477	21/21	0.98	0.06	14,15,17,20	0
4	CAP	E	1477	21/21	0.98	0.06	13,14,15,20	0
3	MG	F	1476	1/1	0.98	0.05	13,13,13,13	0
4	CAP	H	1477	21/21	0.98	0.06	14,14,16,19	0
4	CAP	F	1477	21/21	0.98	0.06	13,15,17,21	0
5	EDO	H	1478	4/4	0.98	0.05	20,20,21,21	0
3	MG	H	1476	1/1	0.99	0.03	13,13,13,13	0
3	MG	C	1476	1/1	0.99	0.04	13,13,13,13	0
3	MG	D	1476	1/1	0.99	0.04	13,13,13,13	0
4	CAP	G	1477	21/21	0.99	0.05	12,14,16,19	0
4	CAP	B	1477	21/21	0.99	0.05	14,14,16,20	0
3	MG	A	1476	1/1	1.00	0.02	13,13,13,13	0
3	MG	B	1476	1/1	1.00	0.04	13,13,13,13	0
3	MG	E	1476	1/1	1.00	0.03	13,13,13,13	0
3	MG	G	1476	1/1	1.00	0.04	12,12,12,12	0

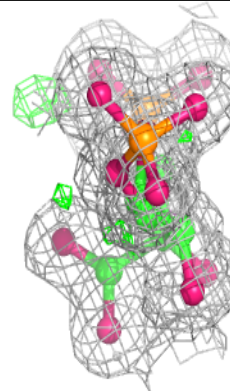
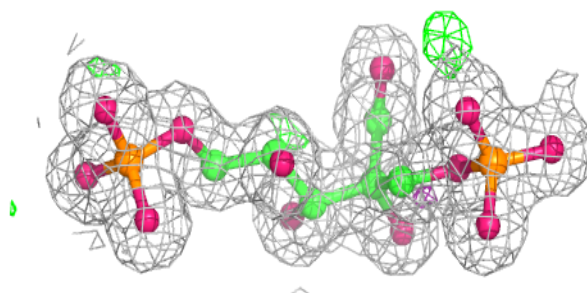
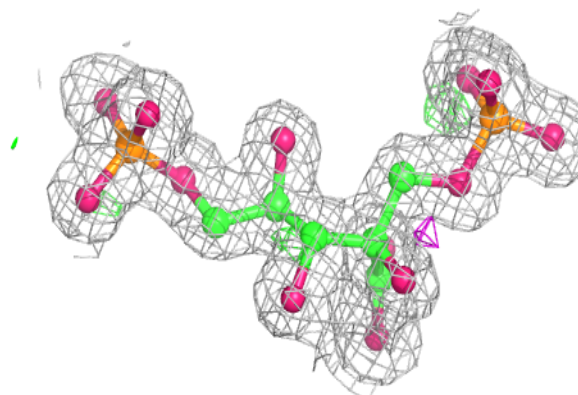
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CAP D 1477:**

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

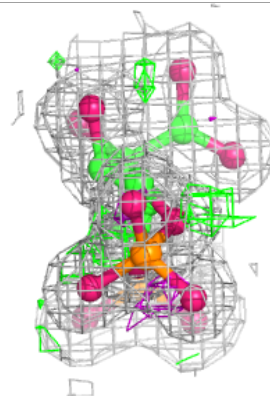
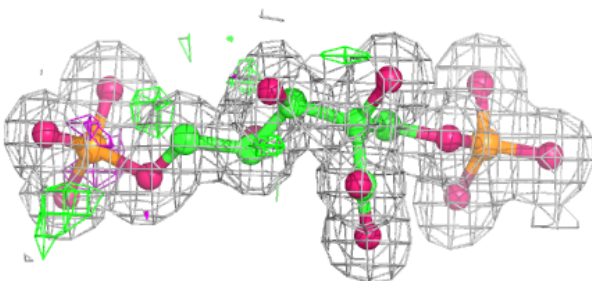
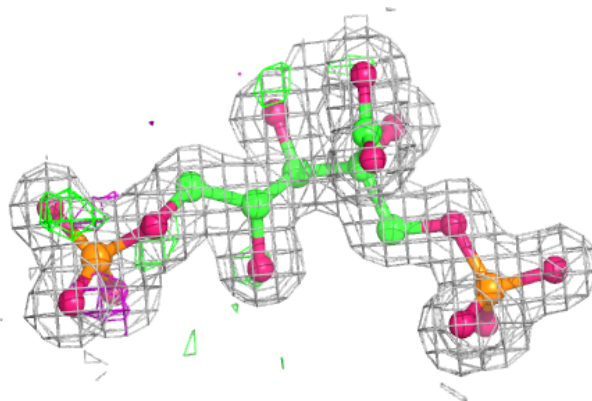
**Electron density around CAP A 1477:**

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

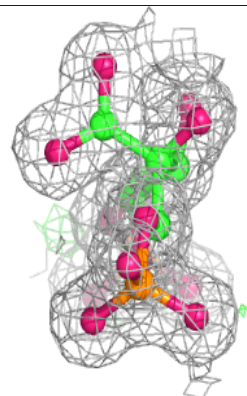
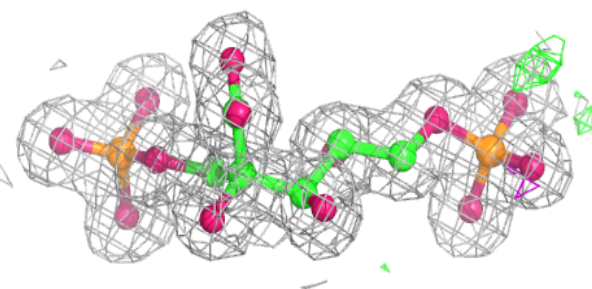
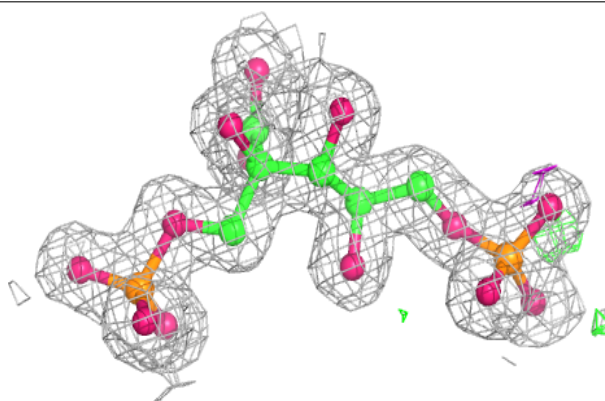


**Electron density around CAP C 1477:**

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

**Electron density around CAP E 1477:**

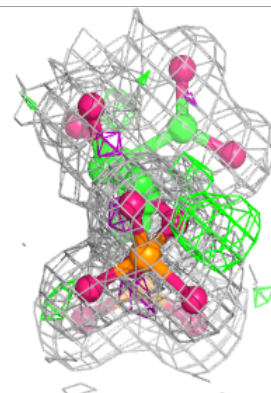
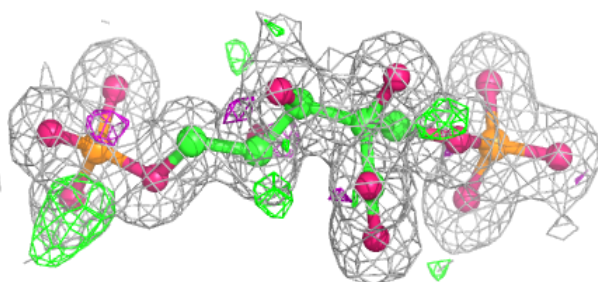
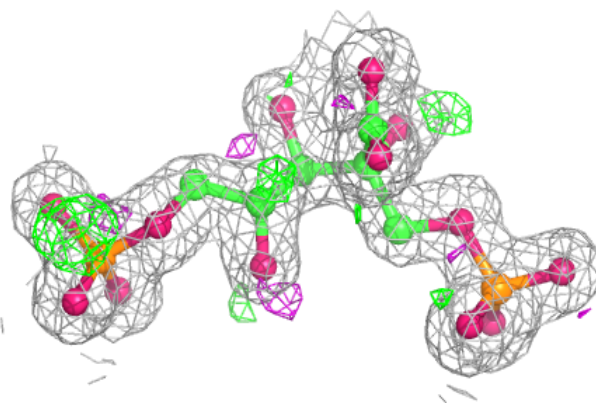
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



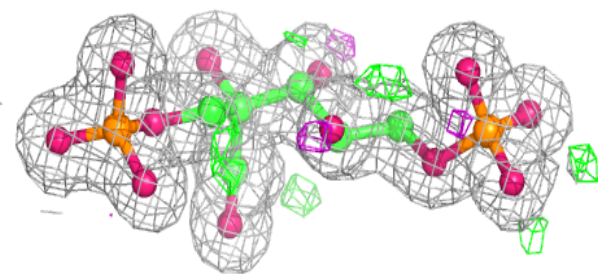
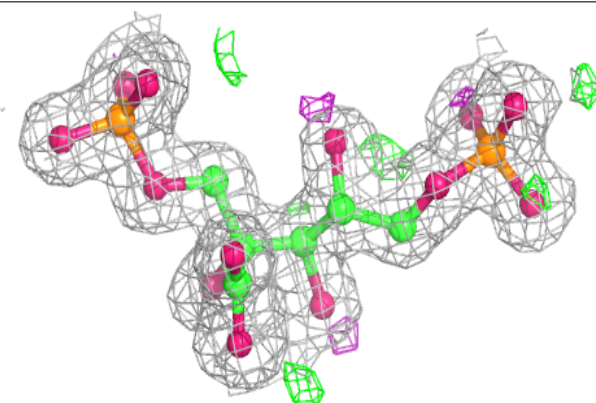


**Electron density around CAP H 1477:**

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

**Electron density around CAP F 1477:**

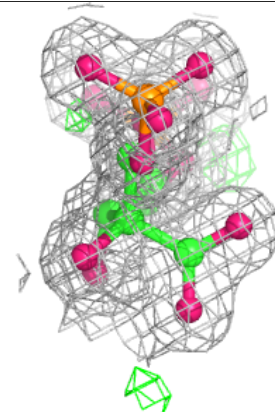
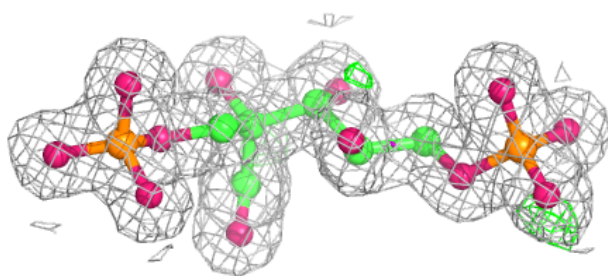
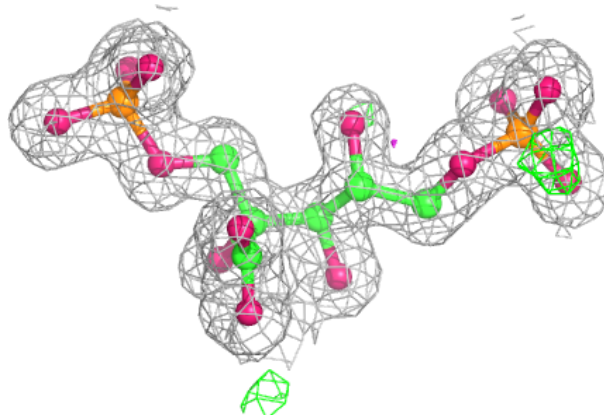
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



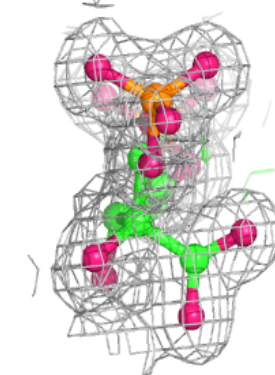
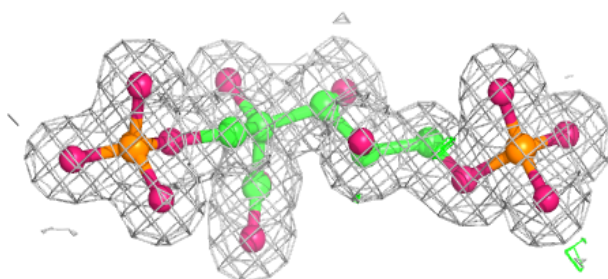
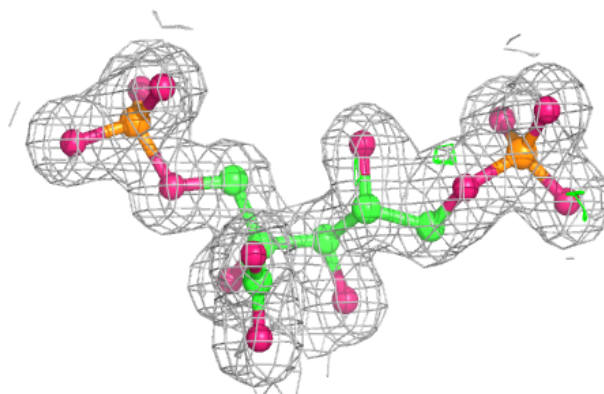


**Electron density around CAP G 1477:**

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

**Electron density around CAP B 1477:**

$2mF_o-DF_c$  (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.