wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2023 – 07:16 am GMT

PDB ID	:	2V67
Title	:	Crystal structure of Chlamydomonas reinhardtii Rubisco with a large- subunit supressor mutation T342I
Authors	:	Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2007-07-13
Resolution	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

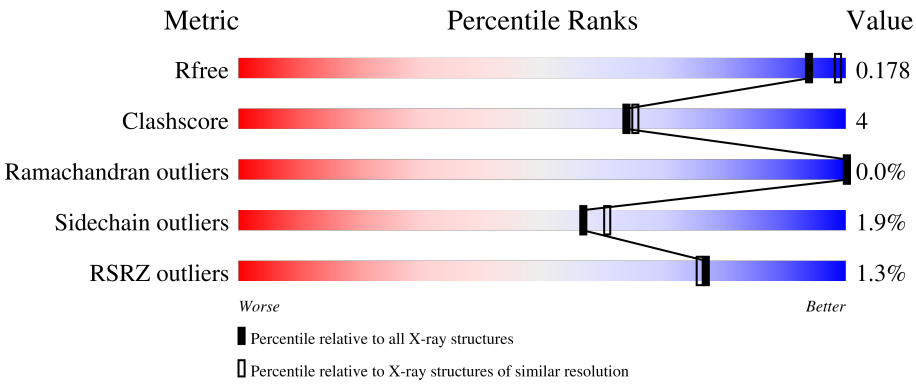
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	.% 89% 8% •
1	B	475	2% 89% 9% •
1	C	475	.% 89% 9% •
1	D	475	.% 88% 10% •
1	E	475	.% 90% 8% •

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Mol	Chain	Length	Quality of chain
1	F	475	2% 88% 9%
1	G	475	.% 89% 9%
1	H	475	.% 88% 10%
2	I	140	3% 85% 13%
2	J	140	2% 89% 9%
2	K	140	89% 10%
2	L	140	85% 14%
2	M	140	88% 11%
2	N	140	.% 89% 10%
2	O	140	.% 89% 9%
2	P	140	2% 85% 14%

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
5	EDO	N	1142	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 41543 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
			Total	C	N	O	S			
1	A	466	3646	2305	642	673	26	0	4	0
1	B	467	3654	2308	643	676	27	0	6	0
1	C	467	3649	2307	643	674	25	0	3	0
1	D	465	3642	2303	641	672	26	0	4	0
1	E	465	3641	2303	641	671	26	0	4	0
1	F	467	3646	2306	640	674	26	0	3	0
1	G	469	3664	2316	646	677	25	0	3	0
1	H	466	3644	2304	642	673	25	0	3	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
A	342	ILE	THR	engineered mutation	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
B	342	ILE	THR	engineered mutation	UNP P00877
C	46	PRO	LEU	conflict	UNP P00877
C	342	ILE	THR	engineered mutation	UNP P00877
D	46	PRO	LEU	conflict	UNP P00877
D	342	ILE	THR	engineered mutation	UNP P00877
E	46	PRO	LEU	conflict	UNP P00877
E	342	ILE	THR	engineered mutation	UNP P00877
F	46	PRO	LEU	conflict	UNP P00877
F	342	ILE	THR	engineered mutation	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
G	46	PRO	LEU	conflict	UNP P00877
G	342	ILE	THR	engineered mutation	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
H	342	ILE	THR	engineered mutation	UNP P00877

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	140	1143	739	190	203	11	0	0	0
2	J	140	1145	740	190	203	12	0	1	0
2	K	140	1145	740	190	203	12	0	1	0
2	L	140	1147	740	193	203	11	0	1	0
2	M	140	1152	743	193	204	12	0	3	0
2	N	140	1143	739	190	203	11	0	0	0
2	O	140	1145	740	190	203	12	0	1	0
2	P	140	1143	739	190	203	11	0	0	0

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

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

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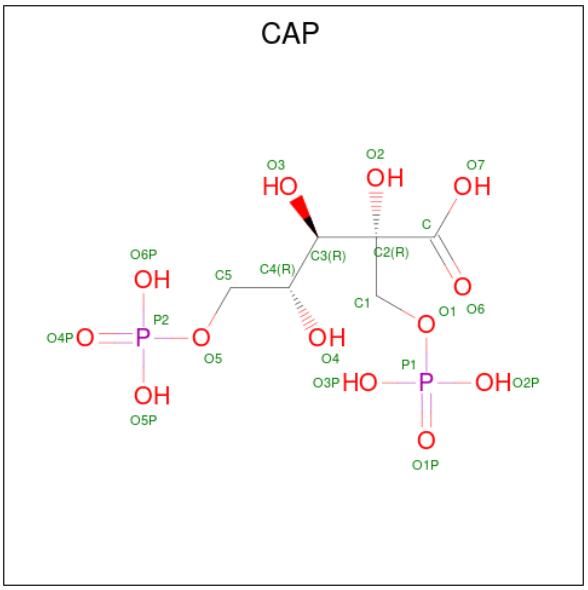
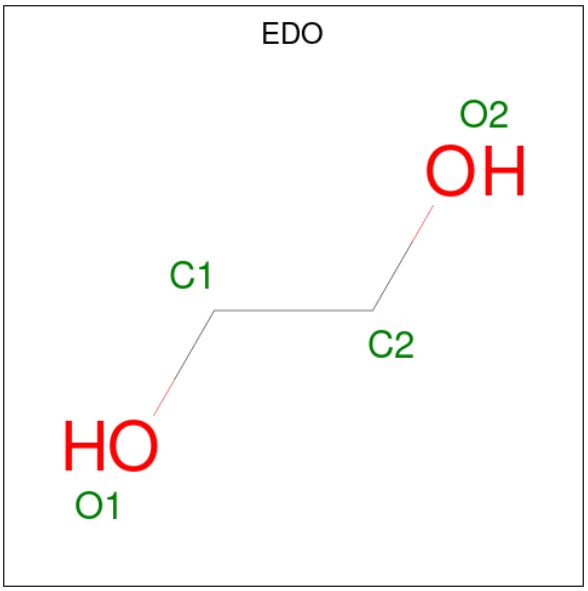
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	H	1	1	1	0	0

- 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
			Total	C	O	P		
4	A	1	21	6	13	2	0	0
			Total	C	O	P		
4	B	1	21	6	13	2	0	0
			Total	C	O	P		
4	C	1	21	6	13	2	0	0
			Total	C	O	P		
4	D	1	21	6	13	2	0	0
			Total	C	O	P		
4	E	1	21	6	13	2	0	0
			Total	C	O	P		
4	F	1	21	6	13	2	0	0
			Total	C	O	P		
4	G	1	21	6	13	2	0	0
			Total	C	O	P		
4	H	1	21	6	13	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0
5	C	1	4	2	2	0	0

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

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

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

- Molecule 6 is water.

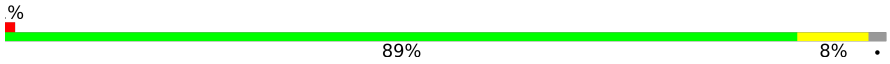
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	287	287	287	0	0
			Total	O		
6	B	272	272	272	0	0
			Total	O		
6	C	274	274	274	0	0
			Total	O		
6	D	269	269	269	0	0
			Total	O		
6	E	266	266	266	0	0
			Total	O		
6	F	241	241	241	0	0
			Total	O		
6	G	271	271	271	0	0
			Total	O		
6	H	273	273	273	0	0
			Total	O		
6	I	77	77	77	0	0
			Total	O		
6	J	78	78	78	0	0
			Total	O		
6	K	90	90	90	0	0
			Total	O		
6	L	84	84	84	0	0
			Total	O		
6	M	98	98	98	0	0
			Total	O		
6	N	64	64	64	0	0
			Total	O		
6	O	71	71	71	0	0
			Total	O		
6	P	71	71	71	0	0

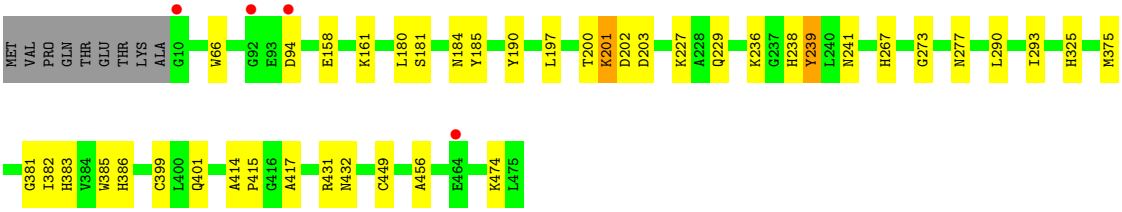
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

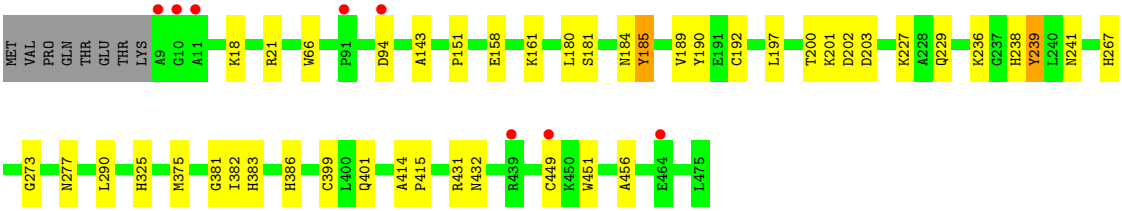
Chain A:





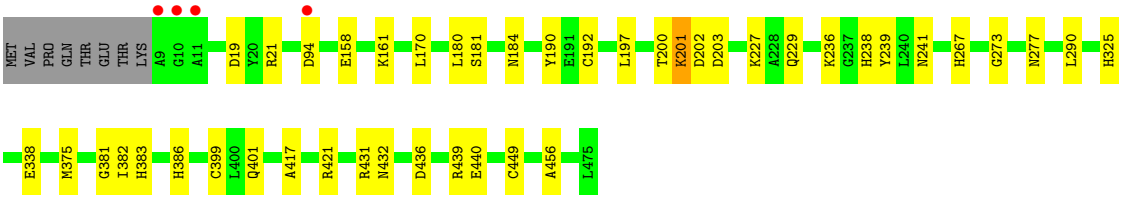
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



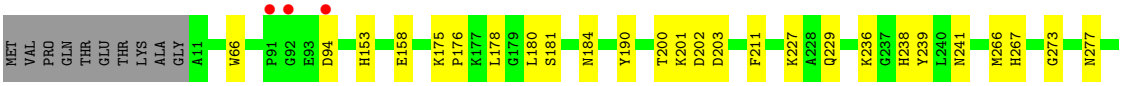
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

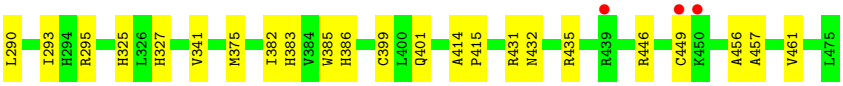
Chain C:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

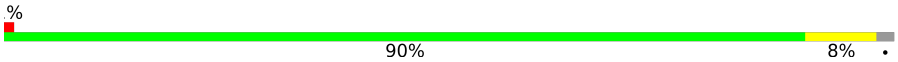
Chain D:

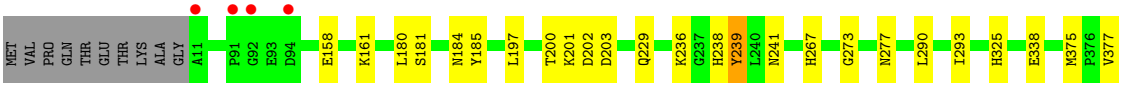




• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

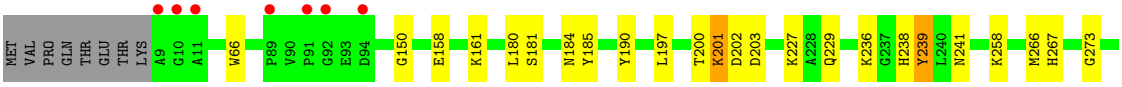
Chain E:

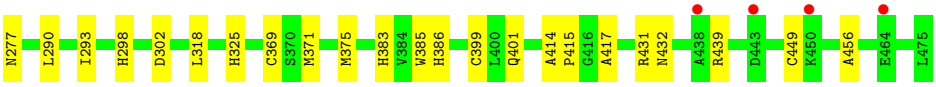




• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

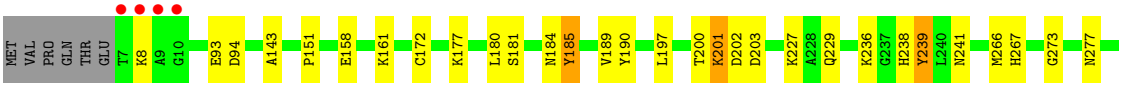
Chain F:

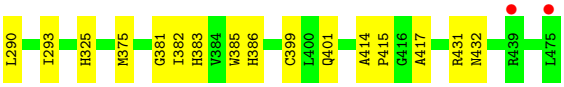




• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

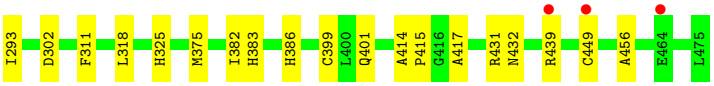
Chain G:





• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

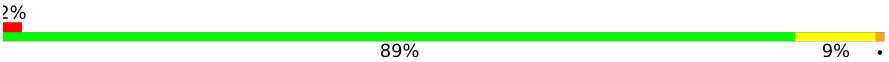
Chain H:

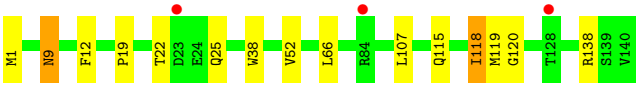


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain I:

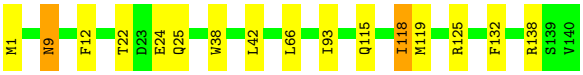
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain J: 



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain K:

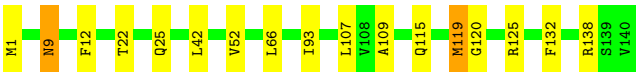


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain L:

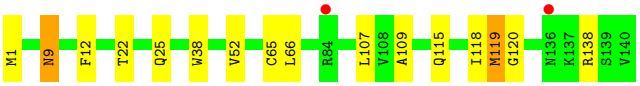
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain M:



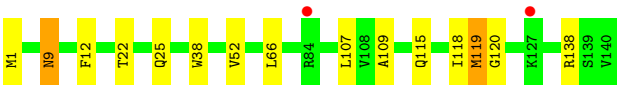
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain N:



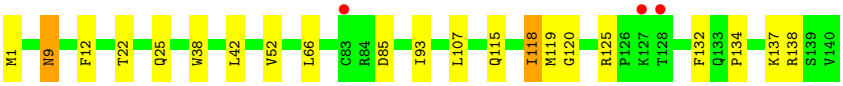
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain O:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P:


M1
N9
F12
T22
Q25
W38
L42
V52
L66
C83
R84
D85
I93
L107
Q115
I118
M119
G120
R125
P126
K127
T128
F132
Q133
P134
K137
R138
S139
V140

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.09Å 178.56Å 122.50Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.00) 89.1 (19.88-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.208 0.177 , 0.178	Depositor DCC
R_{free} test set	13773 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.005 for h,-k,-h-l 0.009 for -h-l,-k,l 0.108 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41543	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CAP, HYP, KCX, EDO, MME, SMC, MG

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	0.41	0/3707	0.54	0/5009
1	B	0.46	0/3727	0.56	0/5036
1	C	0.46	0/3704	0.57	0/5005
1	D	0.45	0/3703	0.56	0/5004
1	E	0.45	0/3702	0.55	0/5004
1	F	0.45	0/3701	0.55	0/5002
1	G	0.45	0/3720	0.56	0/5026
1	H	0.46	0/3699	0.56	0/4998
2	I	0.43	0/1166	0.52	0/1584
2	J	0.44	0/1174	0.55	0/1594
2	K	0.45	0/1174	0.55	0/1594
2	L	0.45	0/1177	0.55	0/1598
2	M	0.44	0/1191	0.54	0/1616
2	N	0.43	0/1166	0.53	0/1584
2	O	0.46	0/1174	0.54	0/1594
2	P	0.46	0/1166	0.56	0/1584
All	All	0.45	0/39051	0.55	0/52832

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3646	0	3553	32	0
1	B	3654	0	3553	37	0
1	C	3649	0	3557	37	0
1	D	3642	0	3550	35	0
1	E	3641	0	3550	28	0
1	F	3646	0	3553	35	0
1	G	3664	0	3573	33	0
1	H	3644	0	3552	32	0
2	I	1143	0	1122	13	0
2	J	1145	0	1123	10	0
2	K	1145	0	1123	11	0
2	L	1147	0	1123	16	0
2	M	1152	0	1133	12	0
2	N	1143	0	1122	11	0
2	O	1145	0	1123	10	0
2	P	1143	0	1122	13	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	8	0	0
4	C	21	0	8	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	8	0	0
5	A	24	0	36	0	0
5	B	20	0	30	2	0
5	C	24	0	36	0	0
5	D	20	0	30	1	0
5	E	24	0	36	2	0
5	F	20	0	30	0	0
5	G	24	0	36	0	0
5	H	20	0	30	0	0
5	I	4	0	6	0	0
5	J	8	0	12	0	0
5	K	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	8	0	12	2	0
5	M	8	0	12	0	0
5	N	8	0	12	0	0
5	O	8	0	12	0	0
5	P	4	0	6	0	0
6	A	287	0	0	3	0
6	B	272	0	0	2	0
6	C	274	0	0	3	0
6	D	269	0	0	6	0
6	E	266	0	0	3	0
6	F	241	0	0	1	0
6	G	271	0	0	2	0
6	H	273	0	0	1	0
6	I	77	0	0	1	0
6	J	78	0	0	0	0
6	K	90	0	0	1	0
6	L	84	0	0	3	0
6	M	98	0	0	0	0
6	N	64	0	0	0	0
6	O	71	0	0	0	0
6	P	71	0	0	1	0
All	All	41543	0	37839	319	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.

The worst 5 of 319 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:375[B]:MET:HE3	1:D:399:CYS:HB2	1.23	1.16
1:H:375[B]:MET:HE3	1:H:399:CYS:HB2	1.28	1.15
1:B:375[B]:MET:HE3	1:B:399:CYS:HB2	1.28	1.15
1:A:375[B]:MET:HE3	1:A:399:CYS:HB2	1.26	1.12
1:C:375[B]:MET:HE3	1:C:399:CYS:HB2	1.24	1.12

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/475 (98%)	451 (97%)	12 (3%)	0	100	100
1	B	466/475 (98%)	454 (97%)	12 (3%)	0	100	100
1	C	463/475 (98%)	450 (97%)	13 (3%)	0	100	100
1	D	462/475 (97%)	450 (97%)	12 (3%)	0	100	100
1	E	462/475 (97%)	448 (97%)	14 (3%)	0	100	100
1	F	463/475 (98%)	449 (97%)	14 (3%)	0	100	100
1	G	465/475 (98%)	451 (97%)	14 (3%)	0	100	100
1	H	462/475 (97%)	450 (97%)	11 (2%)	1 (0%)	47	44
2	I	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
2	J	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	K	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	L	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	M	141/140 (101%)	135 (96%)	6 (4%)	0	100	100
2	N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
2	O	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	P	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
All	All	4817/4920 (98%)	4668 (97%)	148 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	11	ALA

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/376 (99%)	367 (99%)	5 (1%)	69	74
1	B	374/376 (100%)	368 (98%)	6 (2%)	62	67
1	C	371/376 (99%)	368 (99%)	3 (1%)	81	86
1	D	372/376 (99%)	369 (99%)	3 (1%)	81	86
1	E	372/376 (99%)	368 (99%)	4 (1%)	73	78
1	F	371/376 (99%)	366 (99%)	5 (1%)	69	74
1	G	373/376 (99%)	366 (98%)	7 (2%)	57	61
1	H	371/376 (99%)	366 (99%)	5 (1%)	69	74
2	I	122/122 (100%)	116 (95%)	6 (5%)	25	21
2	J	123/122 (101%)	118 (96%)	5 (4%)	30	28
2	K	123/122 (101%)	119 (97%)	4 (3%)	38	37
2	L	123/122 (101%)	118 (96%)	5 (4%)	30	28
2	M	125/122 (102%)	121 (97%)	4 (3%)	39	38
2	N	122/122 (100%)	118 (97%)	4 (3%)	38	37
2	O	123/122 (101%)	119 (97%)	4 (3%)	38	37
2	P	122/122 (100%)	117 (96%)	5 (4%)	30	28
All	All	3959/3984 (99%)	3884 (98%)	75 (2%)	57	61

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	119	MET
2	P	12	PHE
2	M	12	PHE
2	N	119	MET
1	F	241	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	304	GLN
2	N	8	ASN

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Mol	Chain	Res	Type
1	G	432	ASN
2	M	115	GLN
2	O	29	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
2	MME	K	1	2	7,8,9	2.83	1 (14%)	5,8,10	1.33	1 (20%)
1	KCX	E	201	1,3	9,11,12	0.89	0	5,12,14	1.47	1 (20%)
1	SMC	A	369	1	5,6,7	0.76	0	2,6,8	0.75	0
1	SMC	A	256	1	5,6,7	0.58	0	2,6,8	0.19	0
2	MME	I	1	2	7,8,9	2.89	1 (14%)	5,8,10	1.22	1 (20%)
1	HYP	H	151	1	6,8,9	0.68	0	5,10,12	1.46	1 (20%)
1	KCX	H	201	1,3	9,11,12	1.09	1 (11%)	5,12,14	1.57	1 (20%)
1	HYP	F	104	1	6,8,9	0.56	0	5,10,12	1.05	0
2	MME	M	1	2	7,8,9	2.84	1 (14%)	5,8,10	1.42	1 (20%)
1	HYP	E	151	1	6,8,9	0.61	0	5,10,12	1.21	0
1	SMC	E	256	1	5,6,7	0.68	0	2,6,8	0.51	0
1	HYP	C	104	1	6,8,9	0.56	0	5,10,12	1.10	0
1	HYP	H	104	1	6,8,9	0.65	0	5,10,12	1.14	0
1	HYP	F	151	1	6,8,9	0.58	0	5,10,12	1.13	0
1	KCX	F	201	1,3	9,11,12	0.84	0	5,12,14	1.43	1 (20%)
2	MME	O	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.24	1 (20%)
1	SMC	D	369	1	5,6,7	0.83	0	2,6,8	0.74	0
1	SMC	H	256	1	5,6,7	0.64	0	2,6,8	0.84	0
1	SMC	H	369	1	5,6,7	0.91	0	2,6,8	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	E	104	1	6,8,9	0.60	0	5,10,12	0.93	0
1	SMC	F	256	1	5,6,7	0.84	0	2,6,8	0.47	0
1	SMC	F	369	1	5,6,7	1.12	1 (20%)	2,6,8	1.01	0
1	KCX	C	201	1,3	9,11,12	1.08	1 (11%)	5,12,14	1.41	1 (20%)
1	SMC	E	369	1	5,6,7	0.61	0	2,6,8	1.21	0
1	HYP	B	104	1	6,8,9	0.69	0	5,10,12	0.96	0
1	HYP	D	104	1	6,8,9	0.49	0	5,10,12	1.07	0
1	HYP	C	151	1	6,8,9	0.59	0	5,10,12	1.29	0
1	KCX	A	201	1,3	9,11,12	1.03	0	5,12,14	1.57	1 (20%)
1	HYP	A	151	1	6,8,9	0.62	0	5,10,12	1.14	0
1	KCX	B	201	1,3	9,11,12	0.93	0	5,12,14	1.58	1 (20%)
1	SMC	G	256	1	5,6,7	0.55	0	2,6,8	0.28	0
2	MME	P	1	2	7,8,9	2.85	1 (14%)	5,8,10	1.34	1 (20%)
1	KCX	D	201	1,3	9,11,12	0.95	1 (11%)	5,12,14	1.41	1 (20%)
1	HYP	G	151	1	6,8,9	0.56	0	5,10,12	1.30	1 (20%)
1	SMC	B	256	1	5,6,7	0.62	0	2,6,8	0.98	0
2	MME	L	1	2	7,8,9	2.81	1 (14%)	5,8,10	1.22	1 (20%)
1	HYP	A	104	1	6,8,9	0.60	0	5,10,12	1.01	0
1	SMC	G	369	1	5,6,7	0.63	0	2,6,8	0.40	0
1	HYP	B	151	1	6,8,9	0.54	0	5,10,12	1.45	2 (40%)
2	MME	J	1	2	7,8,9	2.94	1 (14%)	5,8,10	1.15	0
1	HYP	D	151	1	6,8,9	0.53	0	5,10,12	1.13	0
1	HYP	G	104	1	6,8,9	0.63	0	5,10,12	1.09	0
1	SMC	B	369	1	5,6,7	0.77	0	2,6,8	1.55	0
1	KCX	G	201	1,3	9,11,12	0.81	0	5,12,14	1.76	1 (20%)
1	SMC	C	256	1	5,6,7	0.55	0	2,6,8	0.60	0
1	SMC	D	256	1	5,6,7	0.94	0	2,6,8	0.67	0
1	SMC	C	369	1	5,6,7	0.70	0	2,6,8	0.92	0
2	MME	N	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.25	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MME	K	1	2	-	2/5/8/10	-
1	KCX	E	201	1,3	-	0/9/10/12	-
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	A	256	1	-	0/3/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MME	I	1	2	-	2/5/8/10	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	H	201	1,3	-	0/9/10/12	-
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
2	MME	M	1	2	-	3/5/8/10	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	SMC	E	256	1	-	0/3/5/7	-
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	1,3	-	0/9/10/12	-
2	MME	O	1	2	-	3/5/8/10	-
1	SMC	D	369	1	-	1/3/5/7	-
1	SMC	H	256	1	-	0/3/5/7	-
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	SMC	F	256	1	-	0/3/5/7	-
1	SMC	F	369	1	-	1/3/5/7	-
1	KCX	C	201	1,3	-	0/9/10/12	-
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,3	-	0/9/10/12	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/9/10/12	-
1	SMC	G	256	1	-	0/3/5/7	-
2	MME	P	1	2	-	3/5/8/10	-
1	KCX	D	201	1,3	-	0/9/10/12	-
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	SMC	B	256	1	-	0/3/5/7	-
2	MME	L	1	2	-	2/5/8/10	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	SMC	G	369	1	-	1/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
2	MME	J	1	2	-	2/5/8/10	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	SMC	B	369	1	-	1/3/5/7	-
1	KCX	G	201	1,3	-	0/9/10/12	-
1	SMC	C	256	1	-	0/3/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	256	1	-	0/3/5/7	-
1	SMC	C	369	1	-	1/3/5/7	-
2	MME	N	1	2	-	2/5/8/10	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	MME	CM-N	-7.49	1.26	1.46
2	I	1	MME	CM-N	-7.39	1.27	1.46
2	K	1	MME	CM-N	-7.35	1.27	1.46
2	N	1	MME	CM-N	-7.34	1.27	1.46
2	O	1	MME	CM-N	-7.31	1.27	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	201	KCX	OQ1-CX-NZ	-3.66	119.29	124.96
1	A	201	KCX	OQ1-CX-NZ	-3.45	119.60	124.96
1	B	201	KCX	OQ1-CX-NZ	-3.41	119.67	124.96
1	H	201	KCX	OQ1-CX-NZ	-3.17	120.05	124.96
1	C	201	KCX	OQ1-CX-NZ	-3.11	120.14	124.96

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	MME	C-CA-CB-CG
2	J	1	MME	C-CA-CB-CG
2	K	1	MME	C-CA-CB-CG
2	M	1	MME	C-CA-CB-CG
2	N	1	MME	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	201	KCX	1	0
1	C	201	KCX	1	0
1	A	201	KCX	1	0
1	G	201	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 74 ligands modelled in this entry, 8 are monoatomic - leaving 66 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	K	1142	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	F	1479	-	3,3,3	0.56	0	2,2,2	0.12	0
5	EDO	H	1479	-	3,3,3	0.51	0	2,2,2	0.29	0
4	CAP	D	477	3	17,20,20	0.85	0	22,31,31	0.86	1 (4%)
5	EDO	E	1480	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	G	1480	-	3,3,3	0.47	0	2,2,2	0.13	0
5	EDO	M	1141	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	F	1476	-	3,3,3	0.43	0	2,2,2	0.51	0
4	CAP	E	477	3	17,20,20	0.81	0	22,31,31	0.80	1 (4%)
5	EDO	C	1481	-	3,3,3	0.53	0	2,2,2	0.10	0
5	EDO	A	1479	-	3,3,3	0.43	0	2,2,2	0.34	0
4	CAP	H	477	3	17,20,20	0.90	0	22,31,31	0.70	0
5	EDO	G	1479	-	3,3,3	0.51	0	2,2,2	0.35	0
5	EDO	C	1480	-	3,3,3	0.49	0	2,2,2	0.36	0
5	EDO	F	1477	-	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	E	1477	-	3,3,3	0.62	0	2,2,2	0.06	0
5	EDO	G	1476	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	M	1142	-	3,3,3	0.50	0	2,2,2	0.16	0
5	EDO	A	1481	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	F	1480	-	3,3,3	0.49	0	2,2,2	0.32	0
4	CAP	F	477	3	17,20,20	0.86	0	22,31,31	0.92	1 (4%)
5	EDO	A	1476	-	3,3,3	0.57	0	2,2,2	0.25	0
5	EDO	D	1479	-	3,3,3	0.61	0	2,2,2	0.08	0
5	EDO	A	1478	-	3,3,3	0.53	0	2,2,2	0.29	0
5	EDO	D	1476	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	E	1479	-	3,3,3	0.48	0	2,2,2	0.38	0
5	EDO	J	1142	-	3,3,3	0.48	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	H	1478	-	3,3,3	0.54	0	2,2,2	0.32	0
5	EDO	H	1480	-	3,3,3	0.45	0	2,2,2	0.32	0
5	EDO	E	1476	-	3,3,3	0.51	0	2,2,2	0.18	0
5	EDO	G	1477	-	3,3,3	0.53	0	2,2,2	0.20	0
5	EDO	B	1479	-	3,3,3	0.51	0	2,2,2	0.29	0
5	EDO	L	1141	-	3,3,3	0.45	0	2,2,2	0.25	0
5	EDO	B	1476	-	3,3,3	0.65	0	2,2,2	0.10	0
5	EDO	I	1141	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	C	1478	-	3,3,3	0.55	0	2,2,2	0.22	0
5	EDO	H	1476	-	3,3,3	0.65	0	2,2,2	0.03	0
5	EDO	B	1477	-	3,3,3	0.45	0	2,2,2	0.29	0
4	CAP	G	477	3	17,20,20	0.85	0	22,31,31	0.78	0
5	EDO	C	1479	-	3,3,3	0.55	0	2,2,2	0.05	0
5	EDO	C	1476	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	B	1480	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	F	1478	-	3,3,3	0.54	0	2,2,2	0.22	0
5	EDO	P	1141	-	3,3,3	0.44	0	2,2,2	0.36	0
4	CAP	B	477	3	17,20,20	0.76	0	22,31,31	0.70	0
5	EDO	D	1480	-	3,3,3	0.42	0	2,2,2	0.49	0
5	EDO	O	1142	-	3,3,3	0.42	0	2,2,2	0.41	0
5	EDO	E	1478	-	3,3,3	0.36	0	2,2,2	0.53	0
5	EDO	L	1142	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	O	1141	-	3,3,3	0.53	0	2,2,2	0.14	0
5	EDO	J	1141	-	3,3,3	0.44	0	2,2,2	0.24	0
4	CAP	C	477	3	17,20,20	0.91	0	22,31,31	0.77	0
5	EDO	K	1141	-	3,3,3	0.50	0	2,2,2	0.19	0
5	EDO	C	1477	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	E	1481	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	N	1142	-	3,3,3	0.53	0	2,2,2	0.21	0
5	EDO	A	1477	-	3,3,3	0.40	0	2,2,2	0.42	0
5	EDO	G	1478	-	3,3,3	0.38	0	2,2,2	0.53	0
5	EDO	N	1141	-	3,3,3	0.48	0	2,2,2	0.37	0
5	EDO	H	1477	-	3,3,3	0.41	0	2,2,2	0.42	0
5	EDO	B	1478	-	3,3,3	0.50	0	2,2,2	0.23	0
5	EDO	D	1477	-	3,3,3	0.50	0	2,2,2	0.24	0
5	EDO	G	1481	-	3,3,3	0.56	0	2,2,2	0.27	0
5	EDO	A	1480	-	3,3,3	0.57	0	2,2,2	0.24	0
5	EDO	D	1478	-	3,3,3	0.54	0	2,2,2	0.07	0
4	CAP	A	477	3	17,20,20	0.83	0	22,31,31	0.77	1 (4%)

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	K	1142	-	-	0/1/1/1	-
5	EDO	F	1479	-	-	0/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
4	CAP	D	477	3	-	7/29/29/29	-
5	EDO	E	1480	-	-	1/1/1/1	-
5	EDO	G	1480	-	-	0/1/1/1	-
5	EDO	M	1141	-	-	0/1/1/1	-
5	EDO	F	1476	-	-	1/1/1/1	-
4	CAP	E	477	3	-	7/29/29/29	-
5	EDO	C	1481	-	-	1/1/1/1	-
5	EDO	A	1479	-	-	0/1/1/1	-
4	CAP	H	477	3	-	6/29/29/29	-
5	EDO	G	1479	-	-	0/1/1/1	-
5	EDO	C	1480	-	-	0/1/1/1	-
5	EDO	F	1477	-	-	0/1/1/1	-
5	EDO	E	1477	-	-	0/1/1/1	-
5	EDO	G	1476	-	-	1/1/1/1	-
5	EDO	M	1142	-	-	1/1/1/1	-
5	EDO	A	1481	-	-	0/1/1/1	-
5	EDO	F	1480	-	-	1/1/1/1	-
4	CAP	F	477	3	-	7/29/29/29	-
5	EDO	A	1476	-	-	0/1/1/1	-
5	EDO	D	1479	-	-	0/1/1/1	-
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	D	1476	-	-	1/1/1/1	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	J	1142	-	-	0/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	H	1480	-	-	1/1/1/1	-
5	EDO	E	1476	-	-	0/1/1/1	-
5	EDO	G	1477	-	-	0/1/1/1	-
5	EDO	B	1479	-	-	0/1/1/1	-
5	EDO	L	1141	-	-	0/1/1/1	-
5	EDO	B	1476	-	-	0/1/1/1	-
5	EDO	I	1141	-	-	0/1/1/1	-
5	EDO	C	1478	-	-	0/1/1/1	-
5	EDO	H	1476	-	-	0/1/1/1	-
5	EDO	B	1477	-	-	1/1/1/1	-
4	CAP	G	477	3	-	7/29/29/29	-
5	EDO	C	1479	-	-	0/1/1/1	-
5	EDO	C	1476	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1480	-	-	1/1/1/1	-
5	EDO	F	1478	-	-	0/1/1/1	-
5	EDO	P	1141	-	-	0/1/1/1	-
4	CAP	B	477	3	-	7/29/29/29	-
5	EDO	D	1480	-	-	1/1/1/1	-
5	EDO	O	1142	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	1/1/1/1	-
5	EDO	L	1142	-	-	1/1/1/1	-
5	EDO	O	1141	-	-	0/1/1/1	-
5	EDO	J	1141	-	-	1/1/1/1	-
4	CAP	C	477	3	-	7/29/29/29	-
5	EDO	K	1141	-	-	0/1/1/1	-
5	EDO	C	1477	-	-	0/1/1/1	-
5	EDO	E	1481	-	-	0/1/1/1	-
5	EDO	N	1142	-	-	1/1/1/1	-
5	EDO	A	1477	-	-	1/1/1/1	-
5	EDO	G	1478	-	-	1/1/1/1	-
5	EDO	N	1141	-	-	0/1/1/1	-
5	EDO	H	1477	-	-	0/1/1/1	-
5	EDO	B	1478	-	-	1/1/1/1	-
5	EDO	D	1477	-	-	1/1/1/1	-
5	EDO	G	1481	-	-	0/1/1/1	-
5	EDO	A	1480	-	-	1/1/1/1	-
5	EDO	D	1478	-	-	0/1/1/1	-
4	CAP	A	477	3	-	7/29/29/29	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	477	CAP	O2-C2-C	-2.92	103.63	108.97
4	D	477	CAP	O2-C2-C	-2.57	104.27	108.97
4	A	477	CAP	O2-C2-C	-2.15	105.04	108.97
4	E	477	CAP	O2-C2-C	-2.07	105.20	108.97

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	477	CAP	O6-C-C2-C1
4	A	477	CAP	O7-C-C2-C1

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Mol	Chain	Res	Type	Atoms
4	A	477	CAP	O6-C-C2-O2
4	A	477	CAP	O7-C-C2-O2
4	A	477	CAP	O3-C3-C4-O4

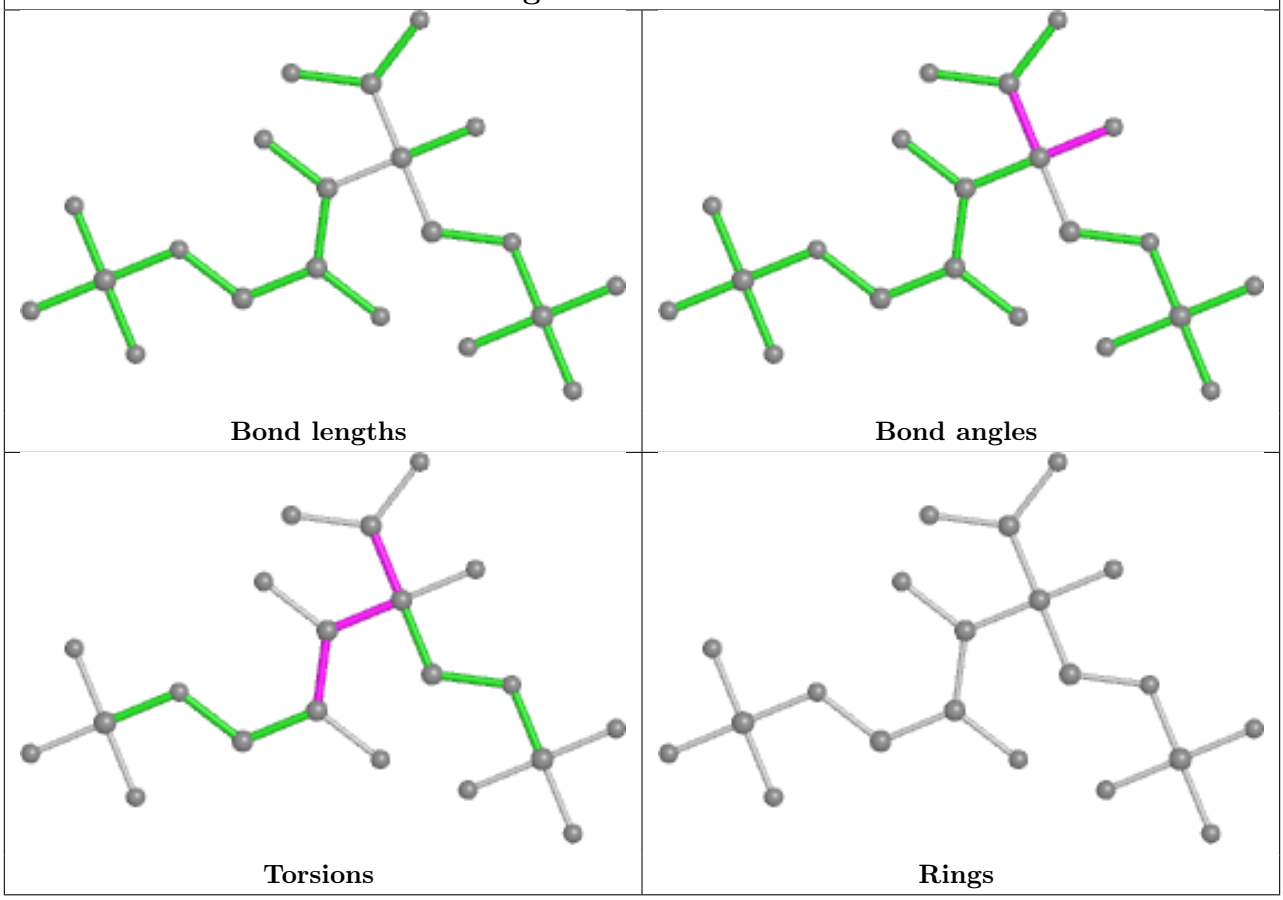
There are no ring outliers.

5 monomers are involved in 7 short contacts:

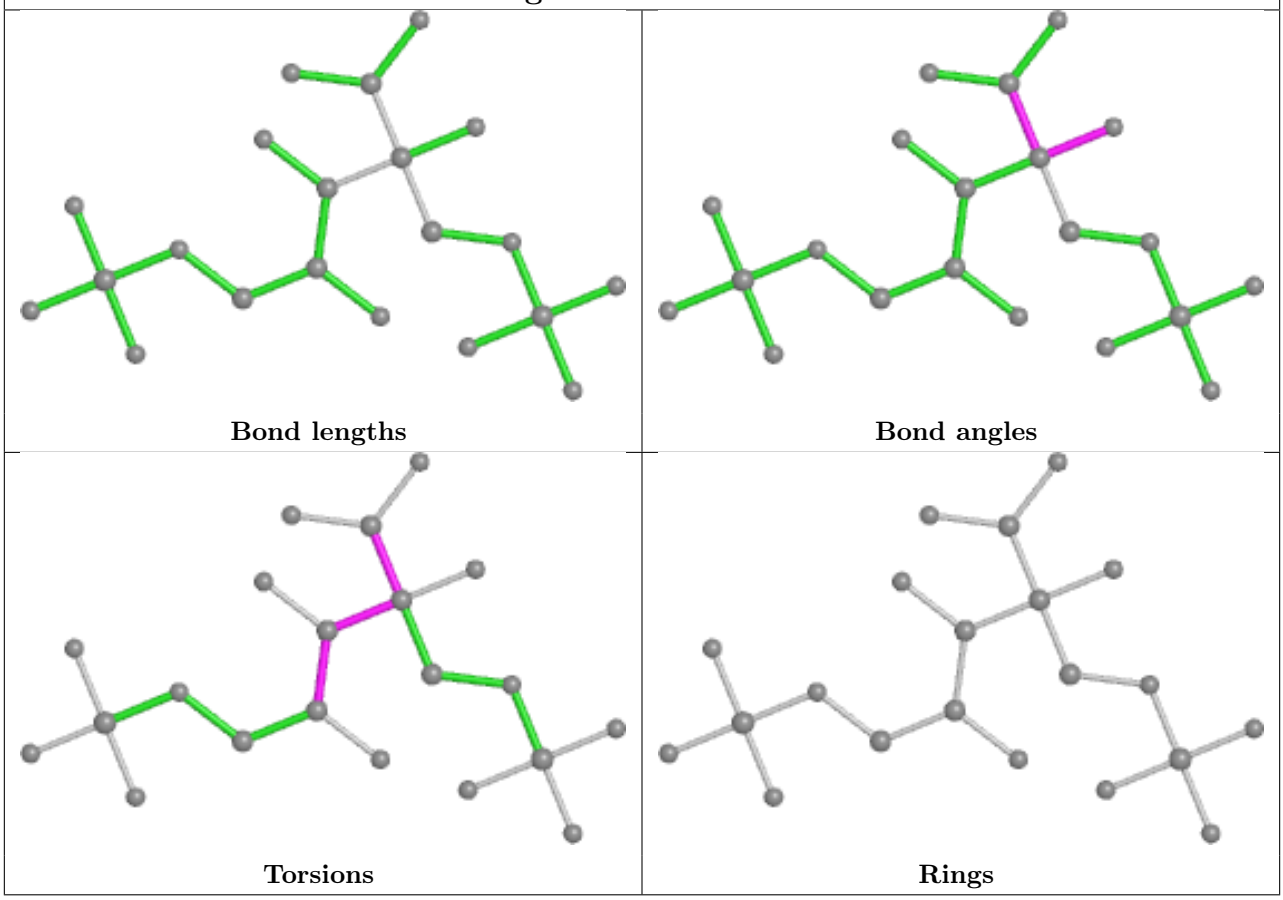
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1480	EDO	2	0
5	L	1141	EDO	2	0
5	B	1477	EDO	1	0
5	B	1480	EDO	1	0
5	D	1480	EDO	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

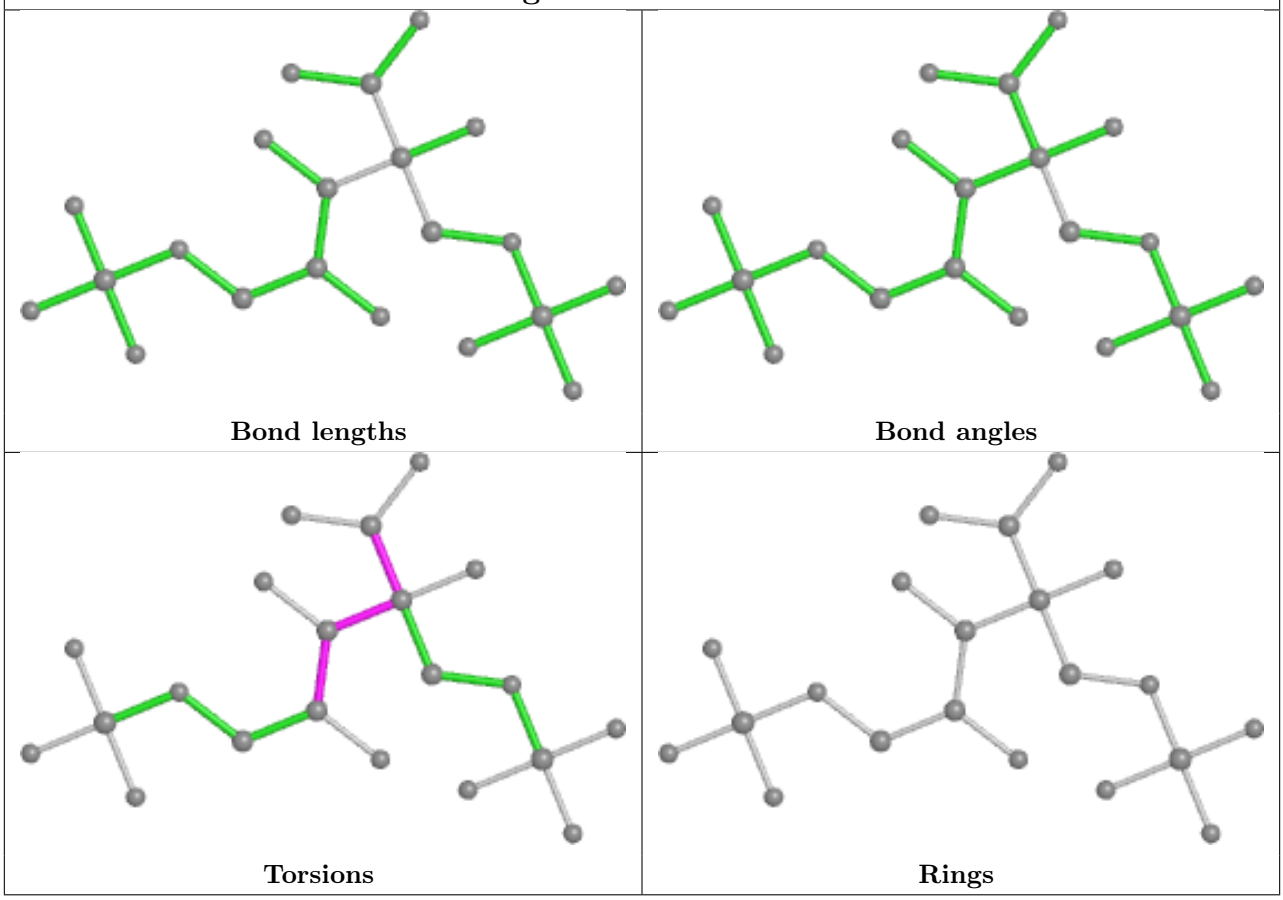
Ligand CAP D 477



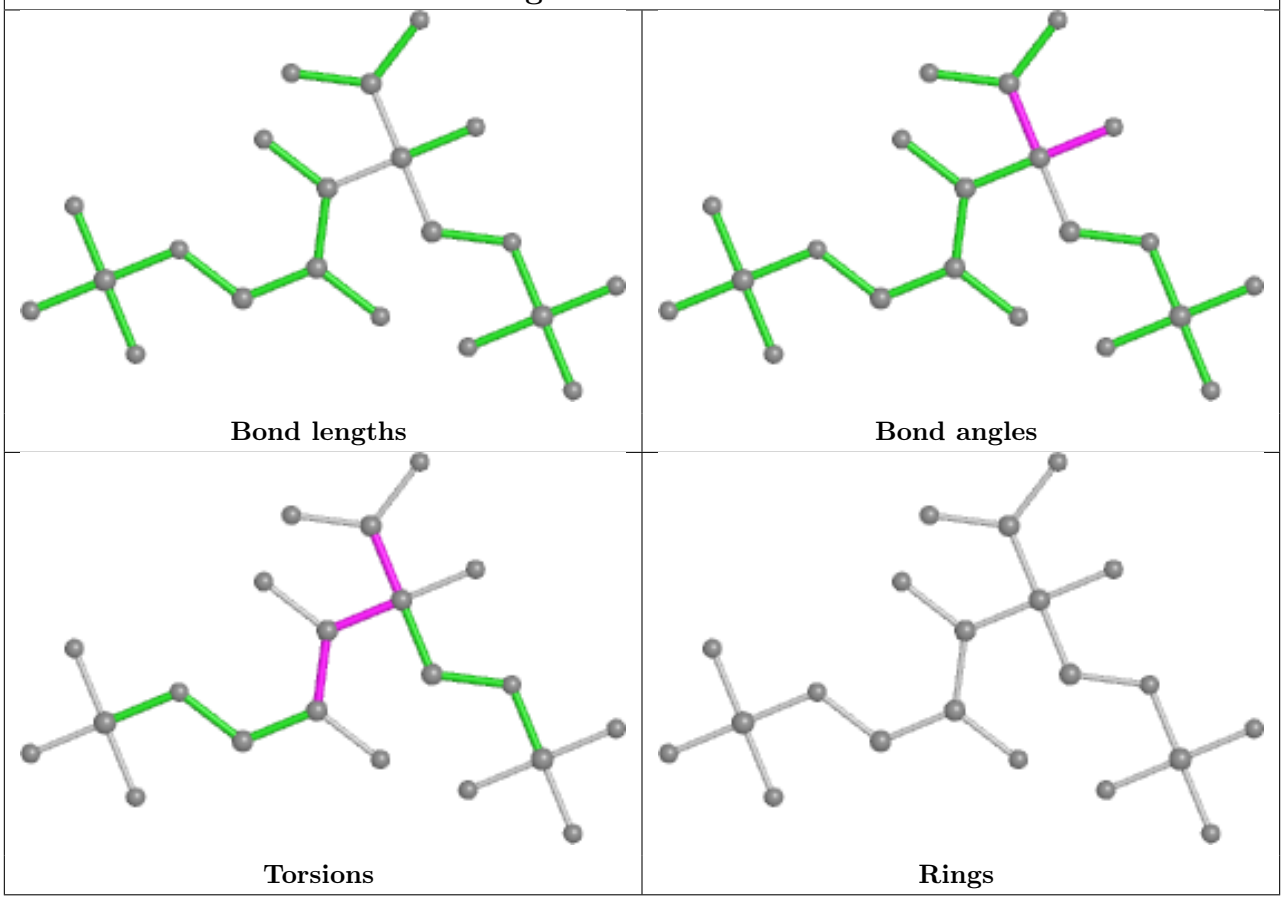
Ligand CAP E 477



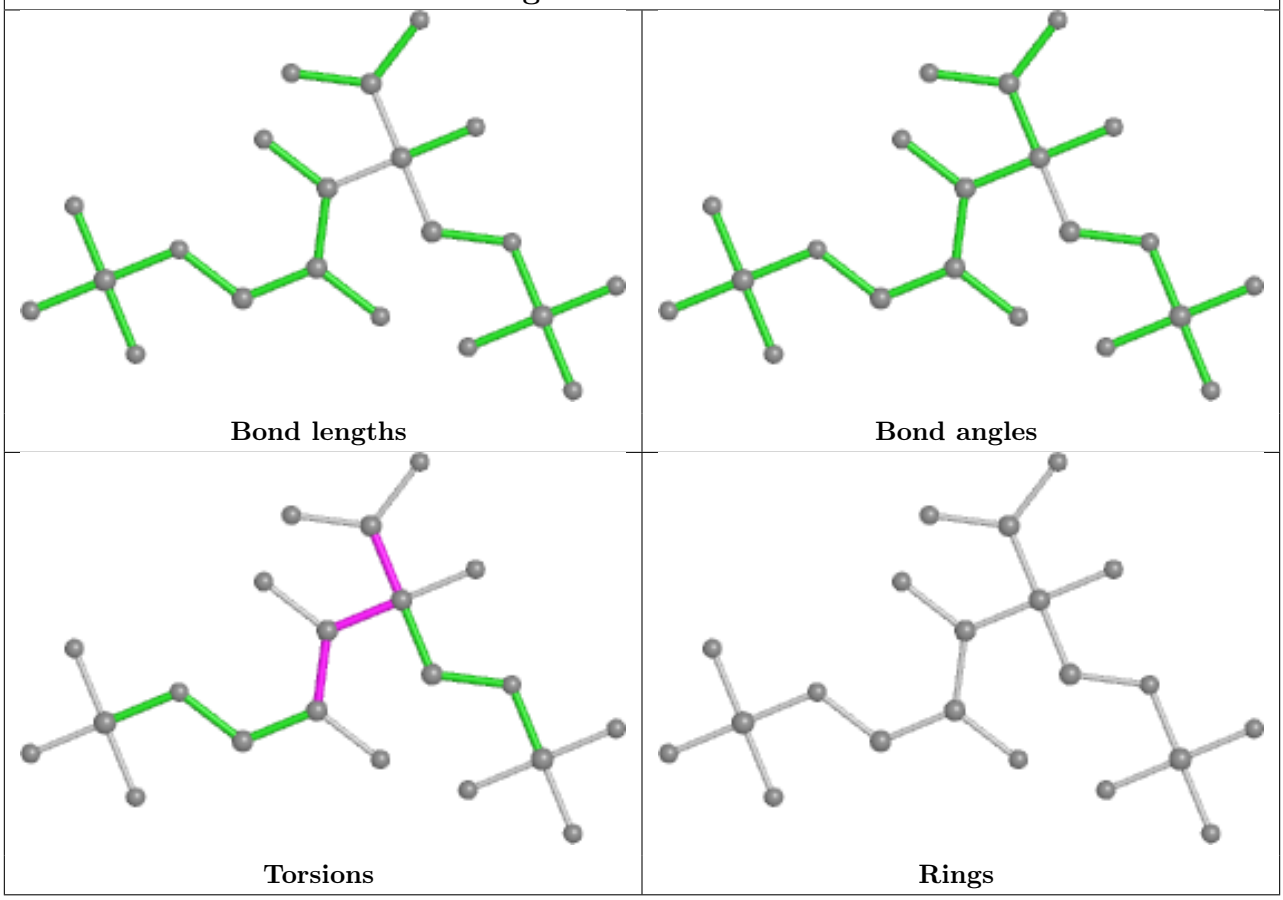
Ligand CAP H 477



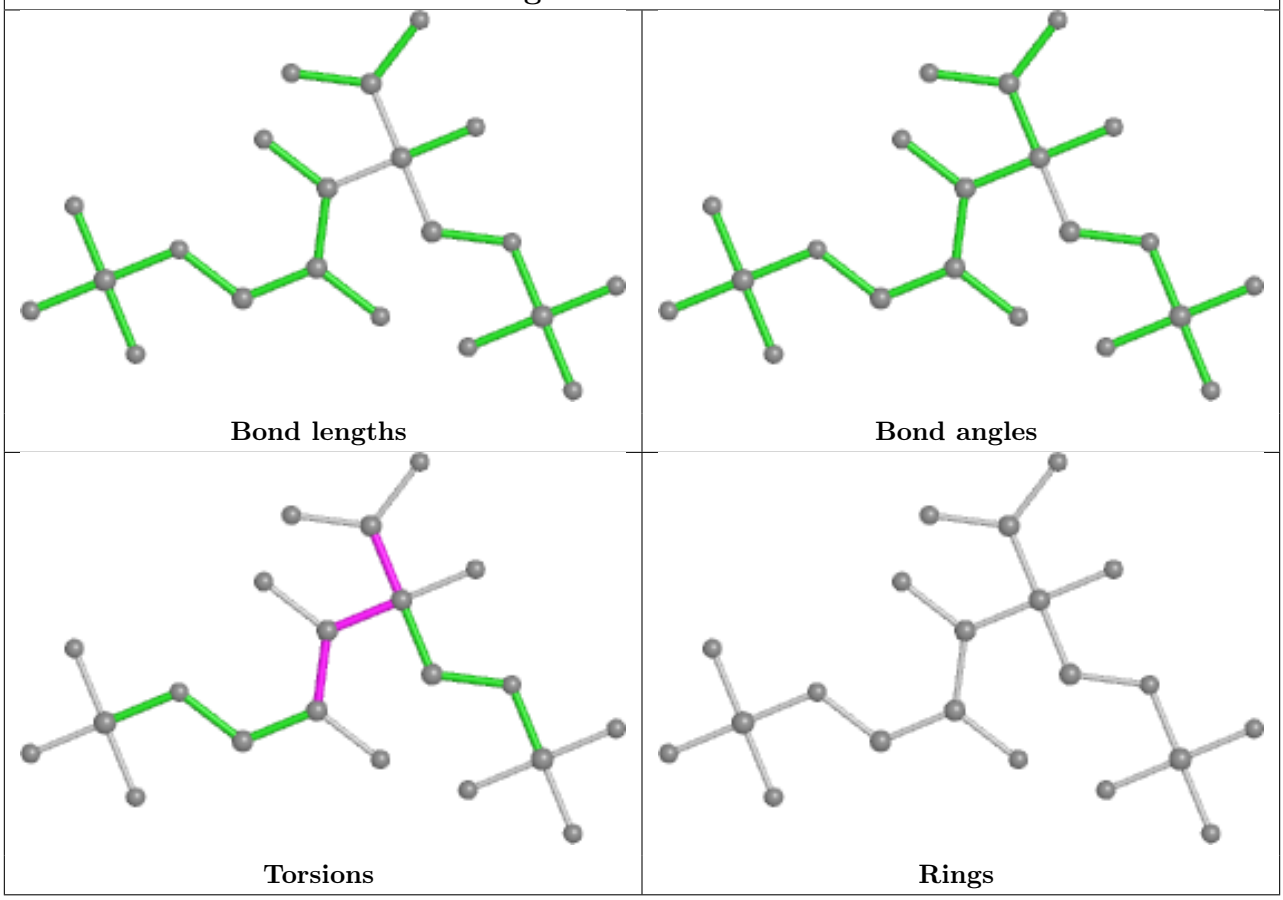
Ligand CAP F 477



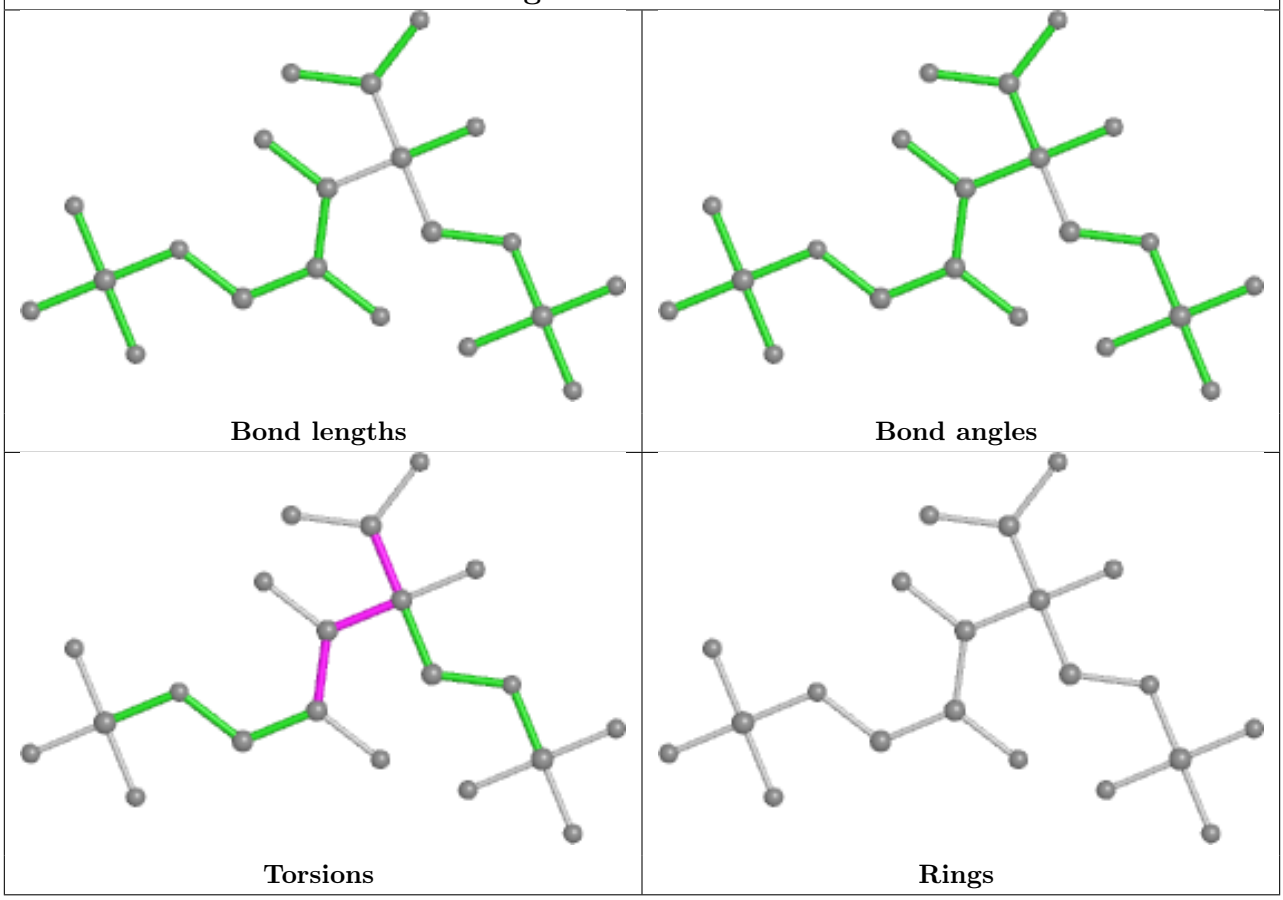
Ligand CAP G 477



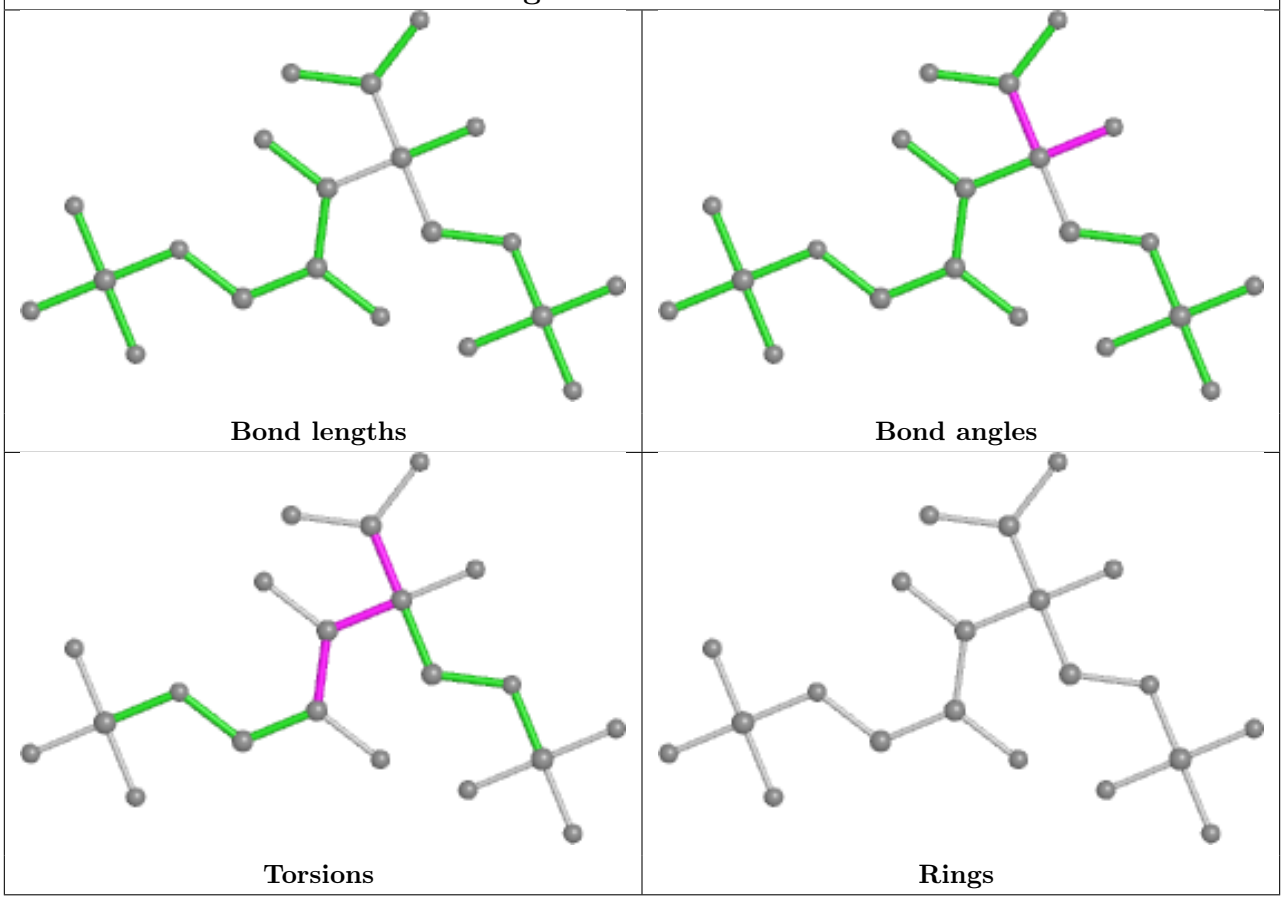
Ligand CAP B 477



Ligand CAP C 477



Ligand CAP A 477



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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^2)	Q<0.9
1	A	461/475 (97%)	-0.56	4 (0%)	84	83	9, 14, 30, 40	0
1	B	462/475 (97%)	-0.58	8 (1%)	70	68	9, 14, 30, 40	0
1	C	462/475 (97%)	-0.57	4 (0%)	84	83	9, 14, 29, 38	0
1	D	460/475 (96%)	-0.59	6 (1%)	77	76	9, 14, 30, 40	0
1	E	460/475 (96%)	-0.58	5 (1%)	80	79	9, 15, 30, 41	0
1	F	462/475 (97%)	-0.53	11 (2%)	59	57	9, 15, 30, 40	1 (0%)
1	G	464/475 (97%)	-0.58	6 (1%)	77	76	9, 14, 30, 51	0
1	H	461/475 (97%)	-0.60	5 (1%)	80	79	9, 14, 30, 42	0
2	I	139/140 (99%)	-0.23	4 (2%)	51	50	12, 20, 33, 36	1 (0%)
2	J	139/140 (99%)	-0.26	3 (2%)	62	60	12, 20, 31, 35	1 (0%)
2	K	139/140 (99%)	-0.32	0	100	100	12, 20, 31, 37	1 (0%)
2	L	139/140 (99%)	-0.36	0	100	100	12, 20, 33, 36	0
2	M	139/140 (99%)	-0.36	0	100	100	12, 19, 30, 33	0
2	N	139/140 (99%)	-0.29	2 (1%)	75	74	12, 20, 35, 41	1 (0%)
2	O	139/140 (99%)	-0.31	2 (1%)	75	74	12, 20, 31, 35	1 (0%)
2	P	139/140 (99%)	-0.26	3 (2%)	62	60	12, 20, 32, 36	1 (0%)
All	All	4804/4920 (97%)	-0.51	63 (1%)	77	76	9, 16, 31, 51	7 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	10	GLY	5.5
1	E	92	GLY	5.1
1	B	9	ALA	4.8
1	G	8	LYS	4.7
1	B	10	GLY	4.5

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, 95th 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^2)	Q<0.9
2	MME	K	1	9/10	0.89	0.15	24,25,33,33	0
2	MME	J	1	9/10	0.90	0.17	24,26,32,33	0
2	MME	O	1	9/10	0.90	0.16	24,25,32,33	0
2	MME	L	1	9/10	0.91	0.17	24,25,32,33	0
2	MME	P	1	9/10	0.91	0.14	24,25,32,33	0
2	MME	M	1	9/10	0.93	0.14	24,25,32,32	0
2	MME	N	1	9/10	0.94	0.20	25,26,33,33	0
2	MME	I	1	9/10	0.95	0.13	24,25,32,33	0
1	HYP	H	151	8/9	0.95	0.08	11,11,12,12	0
1	HYP	A	151	8/9	0.96	0.08	11,12,12,12	0
1	HYP	F	104	8/9	0.96	0.07	11,12,12,13	0
1	SMC	F	369	7/8	0.96	0.09	14,15,16,18	0
1	HYP	A	104	8/9	0.97	0.06	11,11,12,13	0
1	HYP	F	151	8/9	0.97	0.06	11,12,12,12	0
1	KCX	F	201	12/13	0.97	0.07	10,11,11,12	0
1	HYP	B	151	8/9	0.97	0.06	11,12,12,12	0
1	HYP	G	104	8/9	0.97	0.07	11,11,12,12	0
1	HYP	G	151	8/9	0.97	0.07	11,12,12,12	0
1	KCX	G	201	12/13	0.97	0.07	10,10,11,11	0
1	HYP	H	104	8/9	0.97	0.07	11,12,12,13	0
1	SMC	B	369	7/8	0.97	0.06	14,14,16,17	0
1	KCX	H	201	12/13	0.97	0.06	9,11,11,11	0
1	SMC	H	369	7/8	0.97	0.10	14,15,16,18	0
1	HYP	C	104	8/9	0.97	0.07	11,11,12,13	0
1	HYP	C	151	8/9	0.97	0.07	11,12,12,12	0
1	KCX	C	201	12/13	0.97	0.07	10,10,11,12	0
1	HYP	D	104	8/9	0.97	0.08	11,11,12,12	0
1	KCX	D	201	12/13	0.97	0.08	10,11,11,11	0
1	HYP	E	104	8/9	0.97	0.07	11,12,12,13	0
1	HYP	E	151	8/9	0.97	0.07	11,12,12,12	0
1	SMC	E	369	7/8	0.97	0.07	14,14,16,18	0
1	SMC	C	369	7/8	0.98	0.07	14,15,16,18	0
1	SMC	A	369	7/8	0.98	0.08	14,14,16,18	0
1	SMC	H	256	7/8	0.98	0.07	10,10,10,11	0
1	HYP	D	151	8/9	0.98	0.06	11,12,12,12	0
1	HYP	B	104	8/9	0.98	0.06	11,11,12,13	0
1	SMC	F	256	7/8	0.98	0.06	10,10,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SMC	D	256	7/8	0.98	0.08	9,10,10,10	0
1	SMC	D	369	7/8	0.98	0.06	14,14,16,17	0
1	KCX	A	201	12/13	0.98	0.07	9,11,11,11	0
1	KCX	B	201	12/13	0.98	0.07	9,10,11,12	0
1	SMC	G	369	7/8	0.98	0.07	14,14,16,17	0
1	KCX	E	201	12/13	0.98	0.06	9,10,11,11	0
1	SMC	G	256	7/8	0.99	0.06	9,10,10,11	0
1	SMC	B	256	7/8	0.99	0.05	10,10,10,11	0
1	SMC	C	256	7/8	0.99	0.06	9,10,10,11	0
1	SMC	E	256	7/8	0.99	0.06	9,10,10,11	0
1	SMC	A	256	7/8	0.99	0.06	10,10,10,11	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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^2)	Q<0.9
5	EDO	N	1142	4/4	0.22	0.42	54,55,57,57	0
5	EDO	E	1479	4/4	0.67	0.21	49,50,50,50	0
5	EDO	D	1477	4/4	0.67	0.21	42,42,42,44	0
5	EDO	F	1480	4/4	0.72	0.28	49,49,49,49	0
5	EDO	C	1480	4/4	0.73	0.19	48,48,48,48	0
5	EDO	G	1481	4/4	0.77	0.18	37,38,38,38	0
5	EDO	H	1478	4/4	0.78	0.14	38,38,38,38	0
5	EDO	E	1480	4/4	0.78	0.19	37,38,39,41	0
5	EDO	A	1478	4/4	0.79	0.17	40,41,42,43	0
5	EDO	K	1141	4/4	0.79	0.17	31,33,34,37	0
5	EDO	C	1476	4/4	0.79	0.28	45,46,46,47	0
5	EDO	E	1481	4/4	0.83	0.20	45,47,47,48	0
5	EDO	M	1141	4/4	0.83	0.15	47,47,48,48	0
5	EDO	D	1480	4/4	0.83	0.23	47,47,47,48	0
5	EDO	G	1476	4/4	0.85	0.20	41,42,42,43	0
5	EDO	P	1141	4/4	0.85	0.16	38,38,38,40	0
5	EDO	I	1141	4/4	0.86	0.16	35,35,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	F	1477	4/4	0.86	0.13	40,40,41,42	0
5	EDO	L	1142	4/4	0.86	0.20	49,50,51,51	0
5	EDO	A	1479	4/4	0.87	0.20	49,50,50,50	0
5	EDO	M	1142	4/4	0.87	0.19	53,53,53,53	0
5	EDO	L	1141	4/4	0.88	0.18	46,46,46,47	0
5	EDO	F	1479	4/4	0.88	0.14	27,28,29,29	0
5	EDO	E	1477	4/4	0.89	0.12	25,26,27,27	0
5	EDO	B	1480	4/4	0.89	0.17	44,45,45,45	0
5	EDO	J	1142	4/4	0.90	0.13	33,33,34,36	0
5	EDO	B	1478	4/4	0.90	0.11	35,35,35,36	0
5	EDO	C	1479	4/4	0.90	0.32	9,10,10,11	4
5	EDO	J	1141	4/4	0.90	0.13	32,32,32,33	0
5	EDO	D	1478	4/4	0.91	0.14	31,31,31,32	0
5	EDO	B	1479	4/4	0.91	0.15	28,30,31,31	0
5	EDO	H	1476	4/4	0.92	0.10	19,20,21,22	0
5	EDO	G	1480	4/4	0.92	0.32	8,8,8,8	4
5	EDO	B	1476	4/4	0.92	0.12	18,21,22,22	0
5	EDO	C	1477	4/4	0.93	0.09	19,20,21,22	0
5	EDO	H	1480	4/4	0.93	0.22	55,55,55,55	0
5	EDO	O	1142	4/4	0.93	0.11	29,29,30,31	0
5	EDO	K	1142	4/4	0.93	0.10	33,33,34,34	0
5	EDO	F	1478	4/4	0.94	0.16	29,30,30,31	0
5	EDO	O	1141	4/4	0.94	0.12	33,33,33,34	0
5	EDO	C	1478	4/4	0.94	0.10	22,22,22,24	0
5	EDO	N	1141	4/4	0.94	0.10	27,27,27,27	0
5	EDO	F	1476	4/4	0.95	0.09	26,26,27,28	0
5	EDO	E	1478	4/4	0.95	0.13	24,25,26,26	0
5	EDO	D	1476	4/4	0.95	0.09	21,21,23,23	0
5	EDO	G	1479	4/4	0.95	0.14	21,23,23,24	0
5	EDO	H	1479	4/4	0.95	0.15	19,21,21,23	0
5	EDO	B	1477	4/4	0.96	0.07	24,25,25,26	0
5	EDO	C	1481	4/4	0.96	0.15	22,23,24,24	0
5	EDO	D	1479	4/4	0.96	0.09	15,16,16,17	0
5	EDO	G	1478	4/4	0.96	0.09	17,18,18,19	0
5	EDO	A	1476	4/4	0.96	0.09	17,18,18,19	0
5	EDO	A	1477	4/4	0.97	0.08	18,18,19,20	0
3	MG	F	476	1/1	0.97	0.04	11,11,11,11	0
3	MG	G	476	1/1	0.97	0.06	11,11,11,11	0
5	EDO	E	1476	4/4	0.97	0.32	8,8,9,9	4
5	EDO	A	1480	4/4	0.97	0.07	18,19,20,20	0
5	EDO	A	1481	4/4	0.97	0.09	24,25,26,26	0
5	EDO	H	1477	4/4	0.97	0.07	15,17,18,20	0

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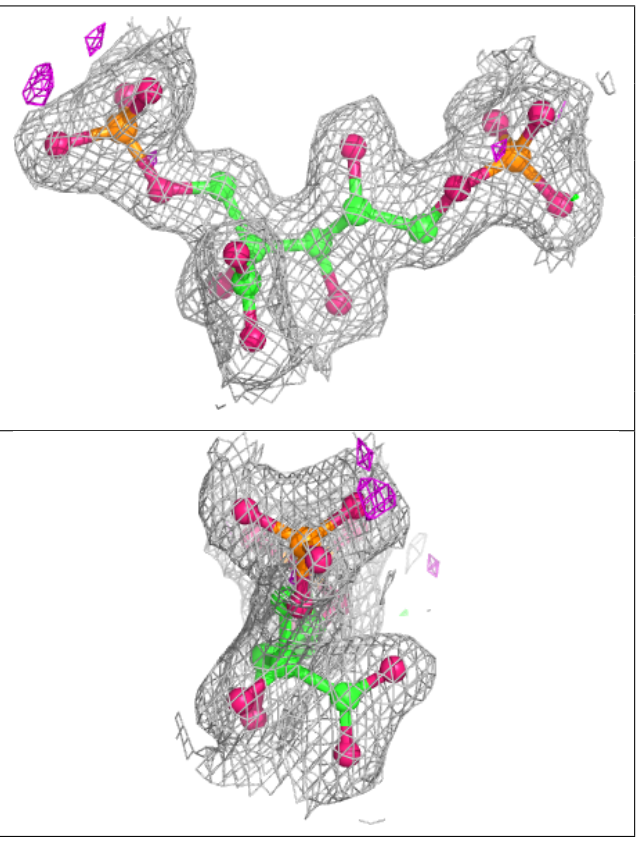
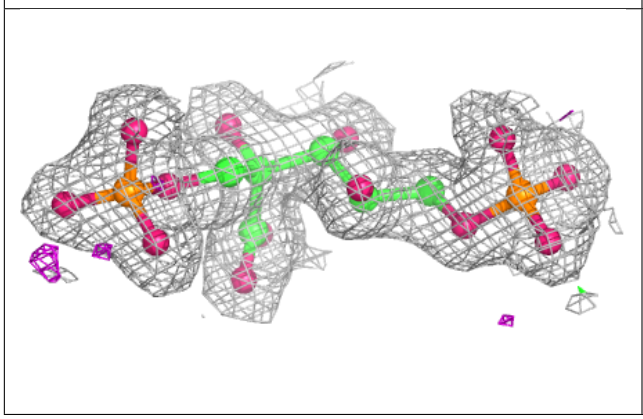
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	E	476	1/1	0.97	0.03	11,11,11,11	0
3	MG	A	476	1/1	0.98	0.06	11,11,11,11	0
4	CAP	B	477	21/21	0.98	0.07	12,15,16,18	0
4	CAP	C	477	21/21	0.98	0.06	11,15,16,18	0
4	CAP	D	477	21/21	0.98	0.06	10,15,15,17	0
4	CAP	E	477	21/21	0.98	0.07	12,15,16,17	0
4	CAP	F	477	21/21	0.98	0.07	13,15,16,18	0
5	EDO	G	1477	4/4	0.98	0.08	18,20,20,21	0
4	CAP	G	477	21/21	0.98	0.06	12,15,16,18	0
4	CAP	H	477	21/21	0.98	0.06	11,15,16,17	0
3	MG	C	476	1/1	0.98	0.05	10,10,10,10	0
3	MG	B	476	1/1	0.99	0.03	10,10,10,10	0
3	MG	H	476	1/1	0.99	0.02	11,11,11,11	0
4	CAP	A	477	21/21	0.99	0.06	12,15,16,18	0
3	MG	D	476	1/1	0.99	0.03	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 B 477:

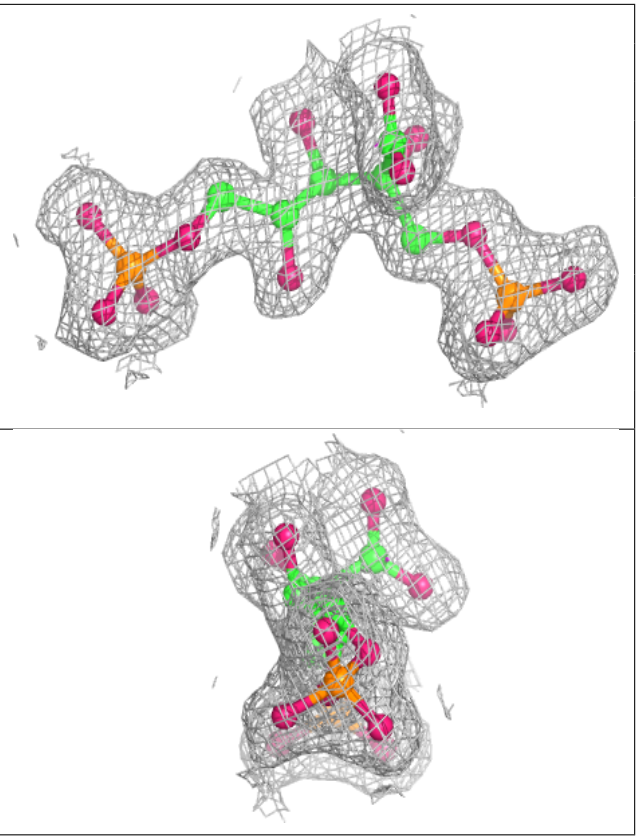
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





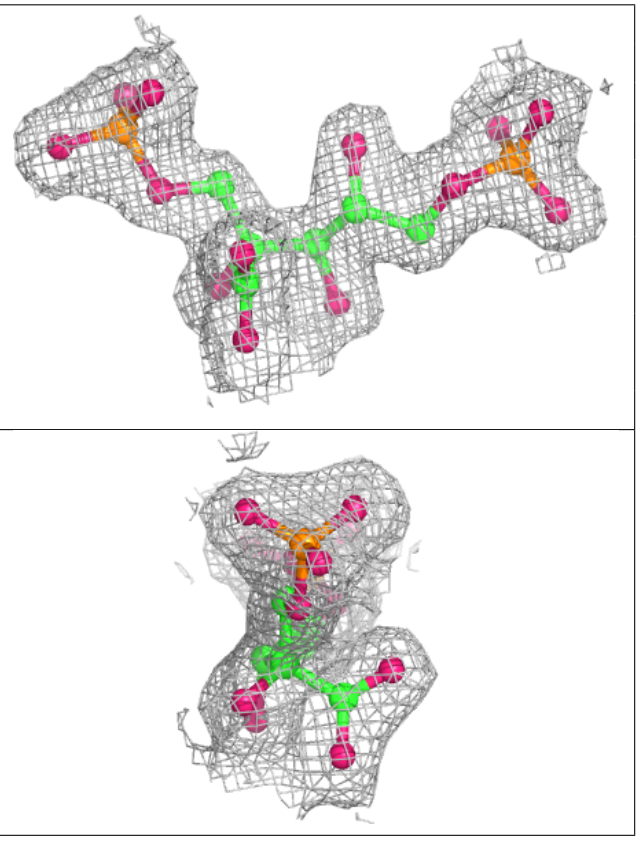
Electron density around CAP C 477:

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



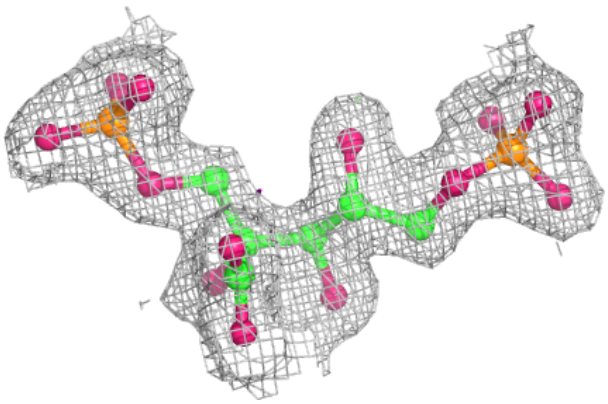
Electron density around CAP D 477:

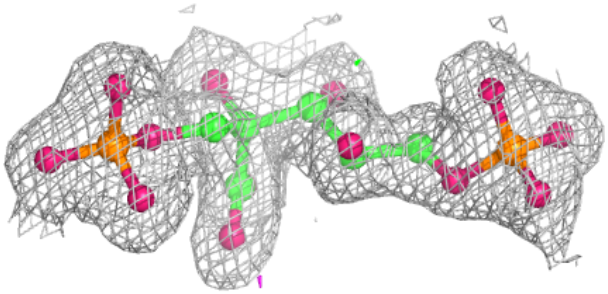
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CAP E 477:

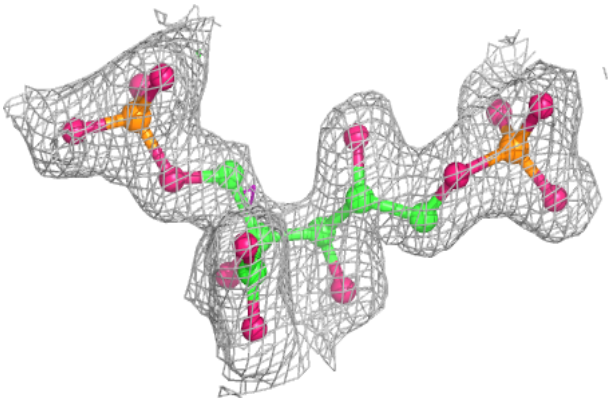
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

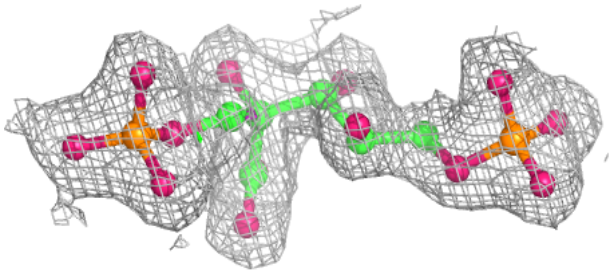


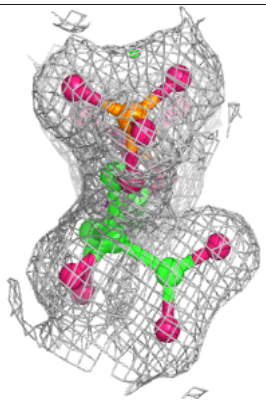


Electron density around CAP F 477:

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

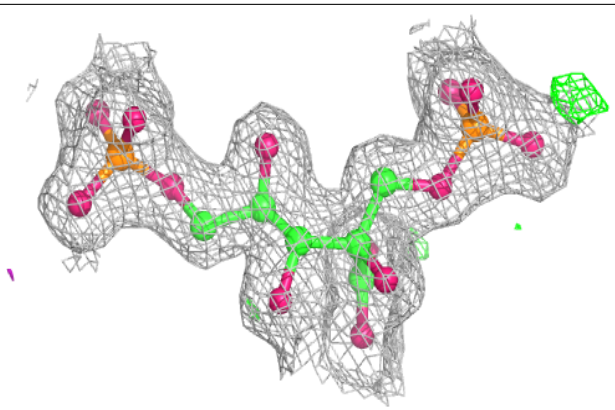


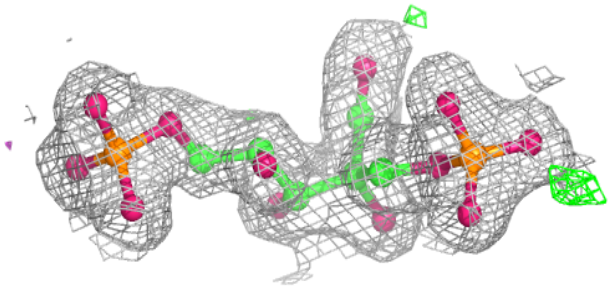


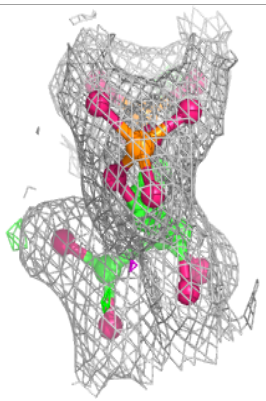


Electron density around CAP G 477:

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

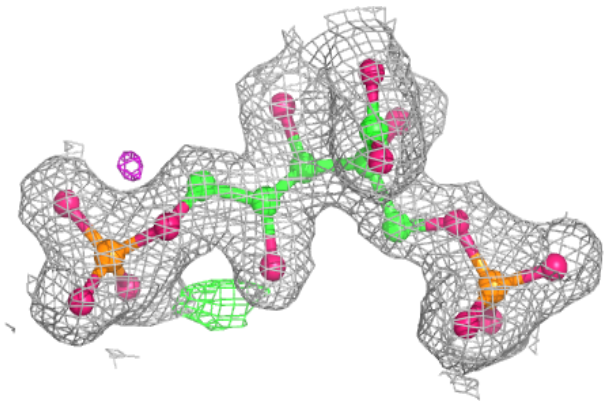


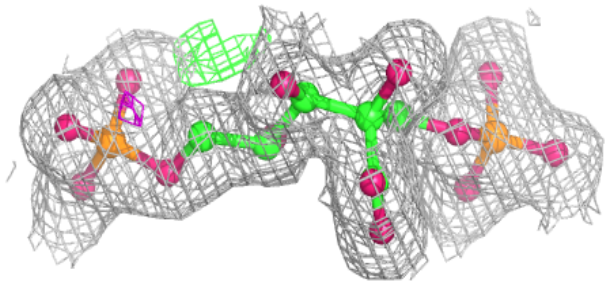


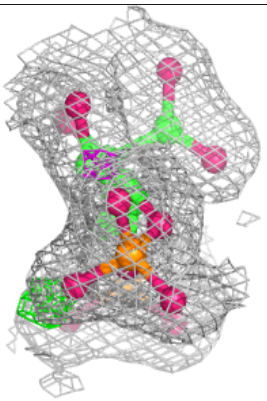


Electron density around CAP H 477:

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

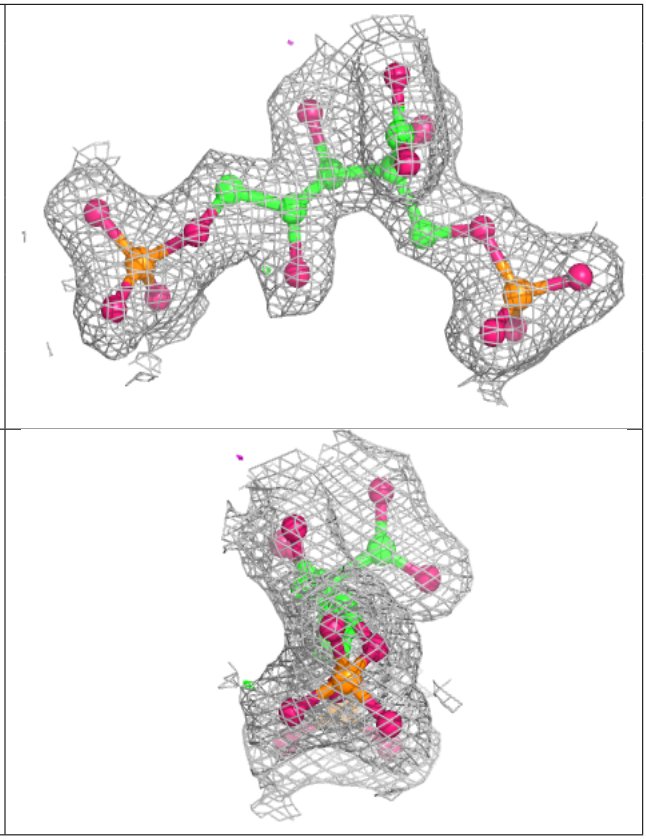






Electron density around CAP A 477:

$2mF_o$-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.