Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 10:20 pm GMT

PDB ID	:	2V63
Title	:	Crystal structure of Rubisco from Chlamydomonas reinhardtii with a large-subunit V331A mutation
Authors	:	Karkehabadi, S.; Satagopagan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2007-07-13
Resolution	:	1.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

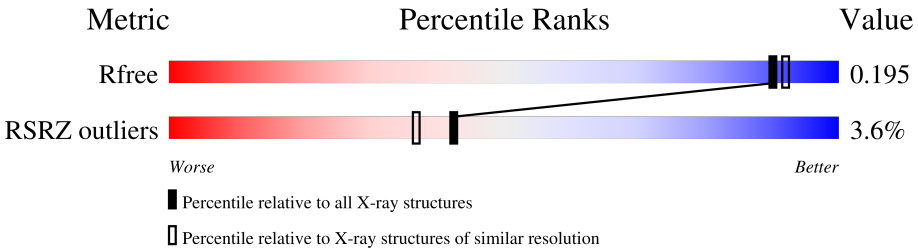
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	C	1477	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 41473 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	466	Total	C	N	O	S	0	4	0
			3643	2302	642	675	24			
1	B	466	Total	C	N	O	S	0	4	0
			3638	2296	642	675	25			
1	C	466	Total	C	N	O	S	0	3	0
			3639	2298	642	675	24			
1	D	464	Total	C	N	O	S	0	2	0
			3626	2291	640	671	24			
1	E	464	Total	C	N	O	S	0	2	0
			3626	2291	640	671	24			
1	F	466	Total	C	N	O	S	0	1	0
			3630	2294	639	673	24			
1	G	466	Total	C	N	O	S	0	2	0
			3634	2295	642	673	24			
1	H	466	Total	C	N	O	S	0	1	0
			3631	2294	641	672	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	variant	UNP P00877
A	331	ALA	VAL	engineered mutation	UNP P00877
B	46	PRO	LEU	variant	UNP P00877
B	331	ALA	VAL	engineered mutation	UNP P00877
C	46	PRO	LEU	variant	UNP P00877
C	331	ALA	VAL	engineered mutation	UNP P00877
D	46	PRO	LEU	variant	UNP P00877
D	331	ALA	VAL	engineered mutation	UNP P00877
E	46	PRO	LEU	variant	UNP P00877
E	331	ALA	VAL	engineered mutation	UNP P00877
F	46	PRO	LEU	variant	UNP P00877
F	331	ALA	VAL	engineered mutation	UNP P00877

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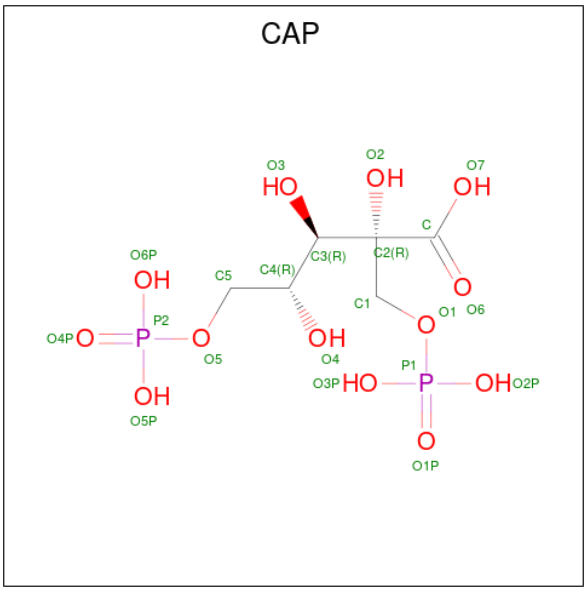
Chain	Residue	Modelled	Actual	Comment	Reference
G	46	PRO	LEU	variant	UNP P00877
G	331	ALA	VAL	engineered mutation	UNP P00877
H	46	PRO	LEU	variant	UNP P00877
H	331	ALA	VAL	engineered mutation	UNP P00877

- 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	0	0
			1143	739	190	203	11			
2	J	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	K	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	L	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	M	140	Total	C	N	O	S	0	2	0
			1146	740	190	204	12			
2	N	140	Total	C	N	O	S	0	1	0
			1144	739	190	204	11			
2	O	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	P	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

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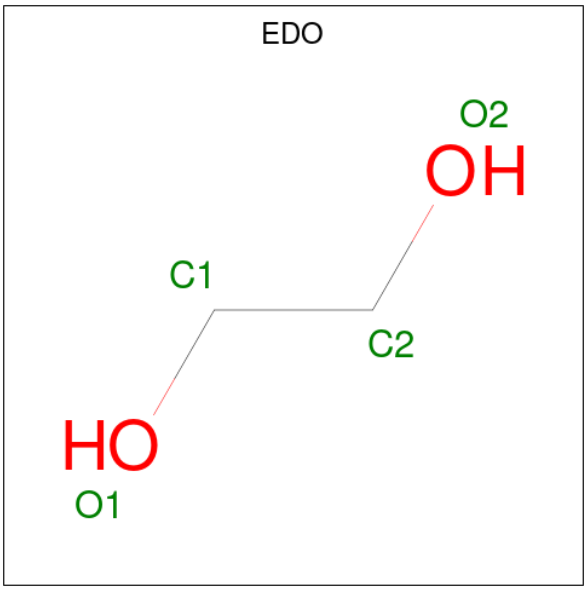
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	296	Total	O	0	0
			296	296		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	287	Total O 287 287	0	0
6	C	282	Total O 282 282	0	0
6	D	262	Total O 262 262	0	0
6	E	262	Total O 262 262	0	0
6	F	253	Total O 253 253	0	0
6	G	287	Total O 287 287	0	0
6	H	281	Total O 281 281	0	0
6	I	75	Total O 75 75	0	0
6	J	84	Total O 84 84	0	0
6	K	91	Total O 91 91	0	0
6	L	96	Total O 96 96	0	0
6	M	106	Total O 106 106	0	0
6	N	72	Total O 72 72	0	0
6	O	81	Total O 81 81	0	0
6	P	77	Total O 77 77	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.38Å 177.45Å 122.57Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-1.80) 92.1 (29.98-1.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.214 0.193 , 0.195	Depositor DCC
R_{free} test set	19570 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h-l,k,h 0.005 for l,k,-h-l 0.016 for h,-k,-h-l 0.014 for -h-l,-k,l 0.196 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41473	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 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	SMC	H	369	1	5,6,7	0.68	0	2,6,8	1.21	0
1	SMC	G	256	1	5,6,7	0.72	0	2,6,8	0.47	0
1	SMC	D	369	1	5,6,7	0.62	0	2,6,8	1.40	0
1	SMC	B	369	1	5,6,7	0.68	0	2,6,8	1.66	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MME	M	1	2	7,8,9	2.90	1 (14%)	5,8,10	1.28	1 (20%)
1	KCX	F	201	1,4	9,11,12	0.89	0	5,12,14	1.64	1 (20%)
2	MME	L	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.30	1 (20%)
1	HYP	D	151	1	6,8,9	0.61	0	5,10,12	1.26	0
1	SMC	A	256	1	5,6,7	0.70	0	2,6,8	0.65	0
1	KCX	H	201	1,4	9,11,12	1.00	1 (11%)	5,12,14	1.54	1 (20%)
1	HYP	C	151	1	6,8,9	0.67	0	5,10,12	1.58	0
1	HYP	E	104	1	6,8,9	0.58	0	5,10,12	1.16	0
1	KCX	G	201	1,4	9,11,12	0.92	0	5,12,14	1.80	1 (20%)
1	HYP	E	151	1	6,8,9	0.61	0	5,10,12	1.53	0
1	HYP	B	151	1	6,8,9	0.60	0	5,10,12	1.52	0
1	KCX	A	201	1,4	9,11,12	1.00	1 (11%)	5,12,14	1.57	1 (20%)
1	SMC	C	256	1	5,6,7	0.51	0	2,6,8	0.80	0
1	KCX	B	201	1,4	9,11,12	0.82	0	5,12,14	1.79	1 (20%)
1	SMC	G	369	1	5,6,7	0.71	0	2,6,8	0.73	0
1	SMC	F	369	1	5,6,7	0.60	0	2,6,8	1.06	0
1	HYP	F	104	1	6,8,9	0.62	0	5,10,12	0.87	0
1	HYP	H	151	1	6,8,9	0.67	0	5,10,12	1.49	0
1	SMC	D	256	1	5,6,7	0.60	0	2,6,8	1.63	0
1	SMC	E	256	1	5,6,7	0.66	0	2,6,8	0.71	0
1	HYP	G	151	1	6,8,9	0.55	0	5,10,12	1.47	0
1	SMC	A	369	1	5,6,7	0.71	0	2,6,8	1.18	0
1	SMC	E	369	1	5,6,7	0.66	0	2,6,8	1.21	0
1	KCX	C	201	1,4	9,11,12	1.02	1 (11%)	5,12,14	1.50	1 (20%)
2	MME	J	1	2	7,8,9	2.88	1 (14%)	5,8,10	1.32	1 (20%)
2	MME	O	1	2	7,8,9	2.89	1 (14%)	5,8,10	1.18	0
1	HYP	C	104	1	6,8,9	0.59	0	5,10,12	0.97	0
1	HYP	A	104	1	6,8,9	0.60	0	5,10,12	0.98	0
1	HYP	A	151	1	6,8,9	0.62	0	5,10,12	1.50	0
1	HYP	B	104	1	6,8,9	0.65	0	5,10,12	0.95	0
1	SMC	C	369	1	5,6,7	0.56	0	2,6,8	0.20	0
1	SMC	B	256	1	5,6,7	0.84	0	2,6,8	0.44	0
2	MME	I	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.30	1 (20%)
2	MME	P	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.31	1 (20%)
2	MME	K	1	2	7,8,9	2.88	1 (14%)	5,8,10	1.36	1 (20%)
2	MME	N	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.30	1 (20%)
1	HYP	D	104	1	6,8,9	0.54	0	5,10,12	1.23	0
1	KCX	E	201	1,4	9,11,12	0.78	0	5,12,14	1.29	1 (20%)
1	HYP	G	104	1	6,8,9	0.64	0	5,10,12	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SMC	F	256	1	5,6,7	0.46	0	2,6,8	1.35	0
1	HYP	F	151	1	6,8,9	0.51	0	5,10,12	1.54	0
1	HYP	H	104	1	6,8,9	0.56	0	5,10,12	1.07	0
1	SMC	H	256	1	5,6,7	0.75	0	2,6,8	0.61	0
1	KCX	D	201	1,4	9,11,12	1.07	0	5,12,14	1.46	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
1	SMC	H	369	1	-	1/3/5/7	-
1	SMC	G	256	1	-	0/3/5/7	-
1	SMC	D	369	1	-	1/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
2	MME	M	1	2	-	3/5/8/10	-
1	KCX	F	201	1,4	-	0/9/10/12	-
2	MME	L	1	2	-	3/5/8/10	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	SMC	A	256	1	-	0/3/5/7	-
1	KCX	H	201	1,4	-	0/9/10/12	-
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	1,4	-	0/9/10/12	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,4	-	0/9/10/12	-
1	SMC	C	256	1	-	0/3/5/7	-
1	KCX	B	201	1,4	-	0/9/10/12	-
1	SMC	G	369	1	-	1/3/5/7	-
1	SMC	F	369	1	-	1/3/5/7	-
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	SMC	D	256	1	-	0/3/5/7	-
1	SMC	E	256	1	-	0/3/5/7	-
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	E	369	1	-	1/3/5/7	-
1	KCX	C	201	1,4	-	1/9/10/12	-
2	MME	J	1	2	-	3/5/8/10	-
2	MME	O	1	2	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	SMC	C	369	1	-	2/3/5/7	-
1	SMC	B	256	1	-	0/3/5/7	-
2	MME	I	1	2	-	3/5/8/10	-
2	MME	P	1	2	-	3/5/8/10	-
2	MME	K	1	2	-	3/5/8/10	-
2	MME	N	1	2	-	3/5/8/10	-
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,4	-	0/9/10/12	-
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	SMC	F	256	1	-	0/3/5/7	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	SMC	H	256	1	-	0/3/5/7	-
1	KCX	D	201	1,4	-	0/9/10/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	MME	CM-N	-7.45	1.27	1.46
2	O	1	MME	CM-N	-7.41	1.27	1.46
2	L	1	MME	CM-N	-7.39	1.27	1.46
2	I	1	MME	CM-N	-7.38	1.27	1.46
2	P	1	MME	CM-N	-7.37	1.27	1.46
2	J	1	MME	CM-N	-7.36	1.27	1.46
2	K	1	MME	CM-N	-7.35	1.27	1.46
2	N	1	MME	CM-N	-7.32	1.27	1.46
1	C	201	KCX	CE-NZ	2.22	1.51	1.46
1	A	201	KCX	CE-NZ	2.02	1.50	1.46
1	H	201	KCX	OQ1-CX	2.00	1.25	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	KCX	OQ1-CX-NZ	-3.98	118.79	124.96
1	G	201	KCX	OQ1-CX-NZ	-3.88	118.95	124.96
1	F	201	KCX	OQ1-CX-NZ	-3.65	119.31	124.96
1	A	201	KCX	OQ1-CX-NZ	-3.47	119.58	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	201	KCX	OQ1-CX-NZ	-3.39	119.70	124.96
1	C	201	KCX	OQ1-CX-NZ	-3.26	119.91	124.96
1	D	201	KCX	OQ1-CX-NZ	-3.22	119.97	124.96
1	E	201	KCX	OQ1-CX-NZ	-2.77	120.66	124.96
2	K	1	MME	CM-N-CA	2.49	121.40	113.64
2	J	1	MME	CM-N-CA	2.41	121.13	113.64
1	B	369	SMC	CA-CB-SG	-2.34	110.25	114.04
2	N	1	MME	CM-N-CA	2.34	120.92	113.64
2	M	1	MME	CM-N-CA	2.34	120.91	113.64
2	L	1	MME	CM-N-CA	2.26	120.69	113.64
2	P	1	MME	CM-N-CA	2.25	120.63	113.64
2	I	1	MME	CM-N-CA	2.20	120.49	113.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	C	369	SMC	N-CA-CB-SG
1	D	369	SMC	N-CA-CB-SG
1	E	369	SMC	N-CA-CB-SG
1	F	369	SMC	N-CA-CB-SG
1	G	369	SMC	N-CA-CB-SG
1	H	369	SMC	N-CA-CB-SG
2	K	1	MME	N-CA-CB-CG
2	P	1	MME	N-CA-CB-CG
1	C	201	KCX	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 8 are monoatomic - leaving 54 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	N	1141	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	B	1478	-	3,3,3	0.48	0	2,2,2	0.23	0
5	EDO	L	1142	-	3,3,3	0.47	0	2,2,2	0.17	0
5	EDO	D	1477	-	3,3,3	0.57	0	2,2,2	0.17	0
5	EDO	F	1476	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	B	1475	-	3,3,3	0.61	0	2,2,2	0.03	0
5	EDO	J	1141	-	3,3,3	0.46	0	2,2,2	0.34	0
3	CAP	D	477	4	17,20,20	0.88	0	22,31,31	0.76	0
5	EDO	N	1142	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	C	1476	-	3,3,3	0.52	0	2,2,2	0.12	0
5	EDO	C	1475	-	3,3,3	0.46	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CAP	C	477	4	17,20,20	0.91	0	22,31,31	0.70	0
5	EDO	G	1478	-	3,3,3	0.51	0	2,2,2	0.27	0
3	CAP	A	476	4	17,20,20	0.88	0	22,31,31	0.66	0
5	EDO	G	1475	-	3,3,3	0.56	0	2,2,2	0.17	0
5	EDO	G	1480	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	J	1142	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	D	1476	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	O	1142	-	3,3,3	0.48	0	2,2,2	0.35	0
3	CAP	G	477	4	17,20,20	0.91	0	22,31,31	0.69	0
5	EDO	H	1477	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	A	1480	-	3,3,3	0.52	0	2,2,2	0.28	0
5	EDO	I	1141	-	3,3,3	0.49	0	2,2,2	0.20	0
5	EDO	P	1141	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	C	1479	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	A	1478	-	3,3,3	0.53	0	2,2,2	0.28	0
5	EDO	G	1479	-	3,3,3	0.51	0	2,2,2	0.13	0
5	EDO	B	1477	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	K	1142	-	3,3,3	0.47	0	2,2,2	0.27	0
3	CAP	B	477	4	17,20,20	0.81	0	22,31,31	0.72	0
3	CAP	E	477	4	17,20,20	0.80	0	22,31,31	0.70	0
5	EDO	G	1476	-	3,3,3	0.44	0	2,2,2	0.29	0
5	EDO	C	1477	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	D	1478	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	C	1478	-	3,3,3	0.55	0	2,2,2	0.23	0
5	EDO	A	1479	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	H	1475	-	3,3,3	0.44	0	2,2,2	0.26	0
5	EDO	L	1141	-	3,3,3	0.45	0	2,2,2	0.20	0
5	EDO	O	1141	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	B	1476	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	M	1141	-	3,3,3	0.44	0	2,2,2	0.29	0
5	EDO	E	1476	-	3,3,3	0.49	0	2,2,2	0.22	0
3	CAP	H	477	4	17,20,20	0.91	0	22,31,31	0.76	0
5	EDO	G	1477	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	K	1141	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	F	1475	-	3,3,3	0.48	0	2,2,2	0.25	0
3	CAP	F	477	4	17,20,20	0.85	0	22,31,31	0.80	1 (4%)
5	EDO	D	1475	-	3,3,3	0.50	0	2,2,2	0.21	0
5	EDO	A	1477	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	E	1475	-	3,3,3	0.53	0	2,2,2	0.22	0
5	EDO	H	1476	-	3,3,3	0.53	0	2,2,2	0.23	0
5	EDO	H	1478	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	M	1142	-	3,3,3	0.50	0	2,2,2	0.16	0
5	EDO	E	1477	-	3,3,3	0.44	0	2,2,2	0.39	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	N	1141	-	-	1/1/1/1	-
5	EDO	B	1478	-	-	0/1/1/1	-
5	EDO	L	1142	-	-	1/1/1/1	-
5	EDO	D	1477	-	-	0/1/1/1	-
5	EDO	F	1476	-	-	0/1/1/1	-
5	EDO	B	1475	-	-	0/1/1/1	-
5	EDO	J	1141	-	-	0/1/1/1	-
3	CAP	D	477	4	-	7/29/29/29	-
5	EDO	N	1142	-	-	0/1/1/1	-
5	EDO	C	1476	-	-	1/1/1/1	-
5	EDO	C	1475	-	-	1/1/1/1	-
3	CAP	C	477	4	-	7/29/29/29	-
5	EDO	G	1478	-	-	1/1/1/1	-
3	CAP	A	476	4	-	7/29/29/29	-
5	EDO	G	1475	-	-	0/1/1/1	-
5	EDO	G	1480	-	-	0/1/1/1	-
5	EDO	J	1142	-	-	0/1/1/1	-
5	EDO	D	1476	-	-	0/1/1/1	-
5	EDO	O	1142	-	-	0/1/1/1	-
3	CAP	G	477	4	-	6/29/29/29	-
5	EDO	H	1477	-	-	0/1/1/1	-
5	EDO	A	1480	-	-	0/1/1/1	-
5	EDO	I	1141	-	-	1/1/1/1	-
5	EDO	P	1141	-	-	0/1/1/1	-
5	EDO	C	1479	-	-	1/1/1/1	-
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	G	1479	-	-	1/1/1/1	-
5	EDO	B	1477	-	-	1/1/1/1	-
5	EDO	K	1142	-	-	0/1/1/1	-
3	CAP	B	477	4	-	7/29/29/29	-
3	CAP	E	477	4	-	7/29/29/29	-
5	EDO	G	1476	-	-	0/1/1/1	-
5	EDO	C	1477	-	-	0/1/1/1	-
5	EDO	D	1478	-	-	0/1/1/1	-
5	EDO	C	1478	-	-	0/1/1/1	-
5	EDO	A	1479	-	-	1/1/1/1	-
5	EDO	H	1475	-	-	1/1/1/1	-
5	EDO	L	1141	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	O	1141	-	-	0/1/1/1	-
5	EDO	B	1476	-	-	1/1/1/1	-
5	EDO	M	1141	-	-	0/1/1/1	-
5	EDO	E	1476	-	-	1/1/1/1	-
3	CAP	H	477	4	-	7/29/29/29	-
5	EDO	G	1477	-	-	0/1/1/1	-
5	EDO	K	1141	-	-	0/1/1/1	-
5	EDO	F	1475	-	-	0/1/1/1	-
3	CAP	F	477	4	-	7/29/29/29	-
5	EDO	D	1475	-	-	1/1/1/1	-
5	EDO	A	1477	-	-	1/1/1/1	-
5	EDO	E	1475	-	-	0/1/1/1	-
5	EDO	H	1476	-	-	0/1/1/1	-
5	EDO	H	1478	-	-	1/1/1/1	-
5	EDO	M	1142	-	-	1/1/1/1	-
5	EDO	E	1477	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	477	CAP	O2-C2-C	-2.14	105.06	108.97

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	476	CAP	O6-C-C2-C1
3	A	476	CAP	O7-C-C2-C1
3	A	476	CAP	O6-C-C2-O2
3	A	476	CAP	O7-C-C2-O2
3	A	476	CAP	O3-C3-C4-O4
3	B	477	CAP	O6-C-C2-C1
3	B	477	CAP	O7-C-C2-C1
3	B	477	CAP	O6-C-C2-O2
3	B	477	CAP	O7-C-C2-O2
3	B	477	CAP	O3-C3-C4-O4
3	C	477	CAP	O6-C-C2-C1
3	C	477	CAP	O7-C-C2-C1
3	C	477	CAP	O6-C-C2-O2
3	C	477	CAP	O7-C-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	477	CAP	O3-C3-C4-O4
3	D	477	CAP	O6-C-C2-C1
3	D	477	CAP	O7-C-C2-C1
3	D	477	CAP	O6-C-C2-O2
3	D	477	CAP	O7-C-C2-O2
3	D	477	CAP	O3-C3-C4-O4
3	E	477	CAP	O6-C-C2-C1
3	E	477	CAP	O7-C-C2-C1
3	E	477	CAP	O6-C-C2-O2
3	E	477	CAP	O7-C-C2-O2
3	E	477	CAP	O3-C3-C4-O4
3	F	477	CAP	O6-C-C2-C1
3	F	477	CAP	O7-C-C2-C1
3	F	477	CAP	O6-C-C2-O2
3	F	477	CAP	O7-C-C2-O2
3	F	477	CAP	O3-C3-C4-O4
3	G	477	CAP	O6-C-C2-C1
3	G	477	CAP	O7-C-C2-C1
3	G	477	CAP	O6-C-C2-O2
3	G	477	CAP	O7-C-C2-O2
3	G	477	CAP	O3-C3-C4-O4
3	H	477	CAP	O6-C-C2-C1
3	H	477	CAP	O7-C-C2-C1
3	H	477	CAP	O6-C-C2-O2
3	H	477	CAP	O7-C-C2-O2
3	H	477	CAP	O3-C3-C4-O4
5	A	1479	EDO	O1-C1-C2-O2
5	C	1479	EDO	O1-C1-C2-O2
5	L	1142	EDO	O1-C1-C2-O2
5	M	1142	EDO	O1-C1-C2-O2
3	A	476	CAP	O2-C2-C3-C4
3	B	477	CAP	O2-C2-C3-C4
3	C	477	CAP	O2-C2-C3-C4
3	D	477	CAP	O2-C2-C3-C4
3	E	477	CAP	O2-C2-C3-C4
3	F	477	CAP	O2-C2-C3-C4
3	G	477	CAP	O2-C2-C3-C4
3	H	477	CAP	O2-C2-C3-C4
3	F	477	CAP	C2-C3-C4-O4
5	A	1477	EDO	O1-C1-C2-O2
5	D	1475	EDO	O1-C1-C2-O2
5	B	1477	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	G	1478	EDO	O1-C1-C2-O2
5	H	1478	EDO	O1-C1-C2-O2
3	C	477	CAP	C2-C3-C4-O4
3	E	477	CAP	C2-C3-C4-O4
3	H	477	CAP	C2-C3-C4-O4
5	E	1476	EDO	O1-C1-C2-O2
5	I	1141	EDO	O1-C1-C2-O2
5	B	1476	EDO	O1-C1-C2-O2
5	C	1475	EDO	O1-C1-C2-O2
5	C	1476	EDO	O1-C1-C2-O2
5	H	1475	EDO	O1-C1-C2-O2
5	L	1141	EDO	O1-C1-C2-O2
3	A	476	CAP	C2-C3-C4-O4
3	B	477	CAP	C2-C3-C4-O4
3	D	477	CAP	C2-C3-C4-O4
5	G	1479	EDO	O1-C1-C2-O2
5	N	1141	EDO	O1-C1-C2-O2
5	E	1477	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

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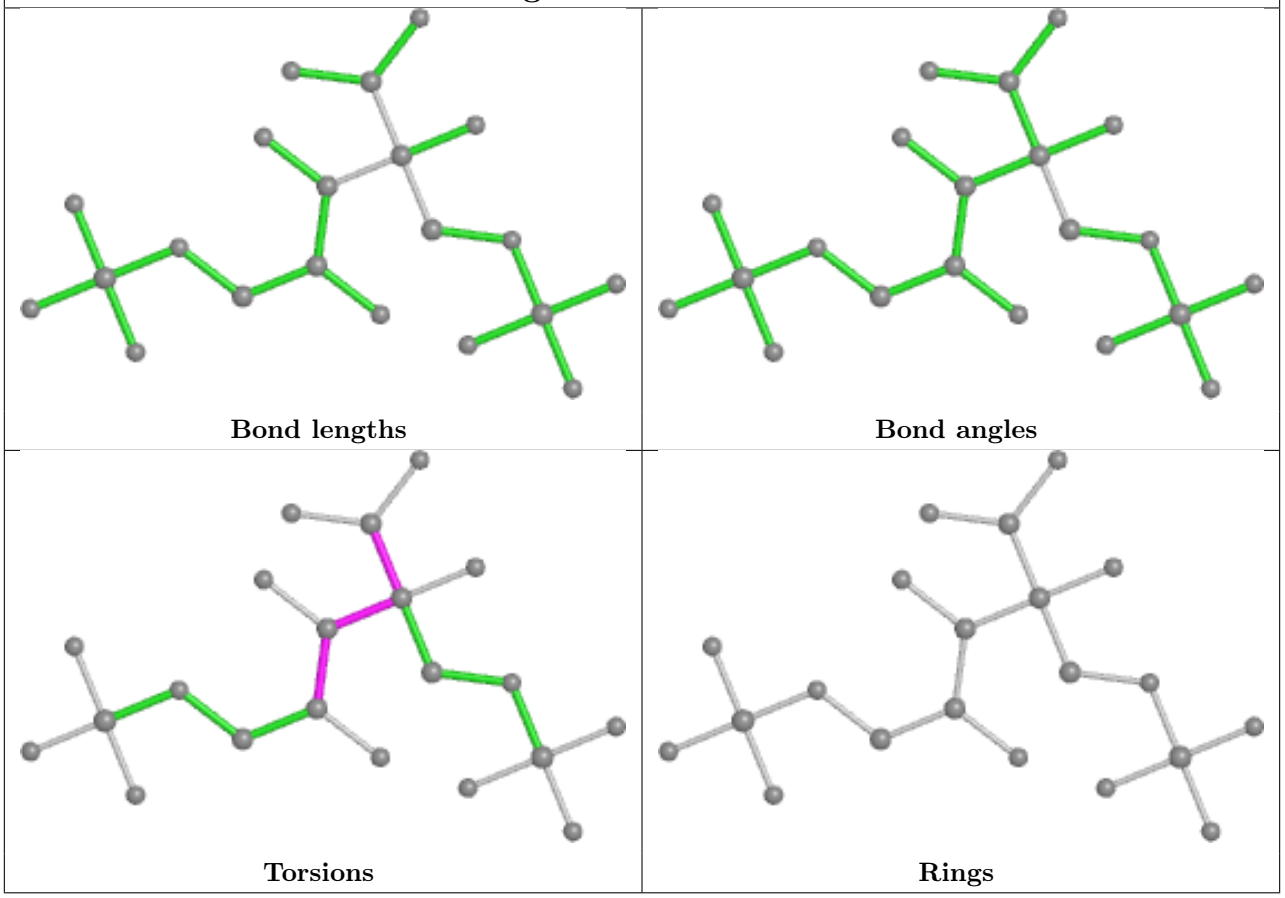

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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^{th} 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%)	0.02	8 (1%) 70 66	5, 12, 25, 37	0
1	B	461/475 (97%)	-0.04	12 (2%) 56 51	5, 12, 25, 37	0
1	C	461/475 (97%)	-0.00	11 (2%) 59 54	5, 12, 25, 37	0
1	D	459/475 (96%)	0.04	15 (3%) 46 40	5, 12, 25, 37	0
1	E	459/475 (96%)	0.08	23 (5%) 28 23	5, 12, 25, 37	0
1	F	461/475 (97%)	0.06	25 (5%) 25 20	5, 12, 26, 37	0
1	G	461/475 (97%)	-0.04	10 (2%) 62 57	5, 11, 25, 37	0
1	H	461/475 (97%)	-0.03	11 (2%) 59 54	5, 12, 25, 37	1 (0%)
2	I	139/140 (99%)	0.39	13 (9%) 8 6	9, 16, 28, 31	0
2	J	139/140 (99%)	0.30	8 (5%) 23 18	9, 17, 28, 31	0
2	K	139/140 (99%)	0.18	3 (2%) 62 57	9, 16, 27, 31	0
2	L	139/140 (99%)	0.14	5 (3%) 42 37	9, 16, 27, 31	0
2	M	139/140 (99%)	0.22	4 (2%) 51 46	9, 16, 26, 31	0
2	N	139/140 (99%)	0.32	8 (5%) 23 18	10, 17, 30, 32	0
2	O	139/140 (99%)	0.24	10 (7%) 15 12	9, 16, 28, 31	0
2	P	139/140 (99%)	0.32	8 (5%) 23 18	10, 17, 27, 31	0
All	All	4796/4920 (97%)	0.07	174 (3%) 42 37	5, 13, 26, 37	1 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	92	GLY	6.9
1	E	94	ASP	6.6
1	E	93	GLU	5.9
1	D	92	GLY	5.2
1	F	94	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	94	ASP	5.0
1	C	11	ALA	4.9
2	I	83	CYS	4.7
2	P	83	CYS	4.6
2	I	128	THR	4.5
2	I	140	VAL	4.4
1	F	91	PRO	4.4
1	D	436	ASP	4.4
1	A	94	ASP	4.3
1	D	94	ASP	4.3
1	C	10	GLY	4.3
1	H	94	ASP	4.3
1	G	11	ALA	4.3
1	F	438	ALA	4.2
1	B	94	ASP	4.1
2	P	128	THR	4.0
1	D	11	ALA	4.0
1	E	11	ALA	4.0
1	F	473	ASP	3.9
2	N	140	VAL	3.9
1	A	92	GLY	3.9
1	F	11	ALA	3.9
2	O	130	ARG	3.8
1	H	9	ALA	3.8
2	N	48	ASP	3.8
1	D	93	GLU	3.8
2	J	128	THR	3.8
1	E	127	PHE	3.6
2	L	140	VAL	3.6
1	H	92	GLY	3.6
1	F	10	GLY	3.5
1	G	10	GLY	3.5
1	F	451	TRP	3.4
1	D	438	ALA	3.4
1	D	91	PRO	3.4
1	E	91	PRO	3.4
2	I	48	ASP	3.4
1	C	9	ALA	3.3
1	D	469	PHE	3.3
1	B	9	ALA	3.3
1	E	438	ALA	3.3
2	J	140	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	434	GLY	3.2
1	E	436	ASP	3.2
2	N	23	ASP	3.2
1	B	10	GLY	3.2
1	D	439	ARG	3.1
1	E	48	VAL	3.1
2	K	140	VAL	3.1
1	F	89	PRO	3.1
1	C	91	PRO	3.1
1	E	470	ASP	3.1
2	J	130	ARG	3.1
1	A	9	ALA	3.0
1	F	392	GLU	3.0
1	F	443	ASP	3.0
1	F	464	GLU	3.0
1	F	9	ALA	2.9
1	G	439	ARG	2.9
2	O	140	VAL	2.9
2	P	48	ASP	2.9
2	M	119	MET	2.9
1	F	439	ARG	2.9
1	B	127	PHE	2.9
1	B	93	GLU	2.8
1	G	94	ASP	2.8
2	O	84	ARG	2.8
1	E	78	ASP	2.8
1	A	464	GLU	2.8
2	J	119	MET	2.8
1	G	9	ALA	2.8
2	J	23	ASP	2.8
2	J	24	GLU	2.8
1	A	473	ASP	2.7
2	M	140	VAL	2.7
2	I	136	ASN	2.7
1	G	127	PHE	2.7
2	L	48	ASP	2.7
1	D	449	CYS	2.7
2	J	102	ASP	2.7
1	D	127	PHE	2.6
1	F	53	CYS	2.6
1	F	450	LYS	2.6
1	F	442	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	439	ARG	2.6
1	B	436	ASP	2.6
2	L	88	GLN	2.6
2	I	137	LYS	2.5
1	B	439	ARG	2.5
2	K	128	THR	2.5
2	N	136	ASN	2.5
2	I	119	MET	2.5
1	C	92	GLY	2.5
1	A	460	GLU	2.5
2	P	119	MET	2.5
1	H	449	CYS	2.5
2	I	135	ALA	2.4
2	O	128	THR	2.4
1	D	89	PRO	2.4
1	F	436	ASP	2.4
1	B	11	ALA	2.4
2	O	127	LYS	2.4
1	G	474	LYS	2.4
2	O	48	ASP	2.4
2	I	2	MET	2.4
2	J	48	ASP	2.4
1	D	443	ASP	2.4
1	C	449	CYS	2.4
1	E	474	LYS	2.3
1	C	473	ASP	2.3
1	E	247	CYS	2.3
2	P	85	ASP	2.3
1	F	441	GLY	2.3
2	N	21	LEU	2.3
1	F	93	GLU	2.3
1	H	93	GLU	2.3
1	C	451	TRP	2.3
2	O	119	MET	2.3
2	O	113	GLN	2.3
1	D	470	ASP	2.3
1	H	460	GLU	2.2
2	O	23	ASP	2.2
1	E	88	GLU	2.2
2	I	84	ARG	2.2
2	O	102	ASP	2.2
1	B	451	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	450	LYS	2.2
1	F	471	THR	2.2
1	G	438	ALA	2.2
1	H	438	ALA	2.2
1	A	451	TRP	2.2
1	B	449	CYS	2.2
1	H	127	PHE	2.2
1	H	28	ASP	2.2
2	N	24	GLU	2.2
1	E	472	ILE	2.2
1	E	450	LYS	2.2
1	F	92	GLY	2.2
2	N	84	ARG	2.2
2	P	23	ASP	2.2
1	H	443	ASP	2.1
2	I	127	LYS	2.1
2	K	127	LYS	2.1
1	E	89	PRO	2.1
1	F	449	CYS	2.1
2	P	24	GLU	2.1
1	F	47	GLY	2.1
1	E	47	GLY	2.1
1	A	93	GLU	2.1
1	C	443	ASP	2.1
1	G	436	ASP	2.1
2	L	102	ASP	2.1
2	N	88	GLN	2.1
1	E	28	ASP	2.0
1	G	464	GLU	2.0
1	B	438	ALA	2.0
2	I	130	ARG	2.0
1	E	33	ASP	2.0
1	F	399	CYS	2.0
1	B	92	GLY	2.0
1	H	464	GLU	2.0
1	E	473	ASP	2.0
2	I	85	ASP	2.0
2	M	102	ASP	2.0
2	L	119	MET	2.0
2	P	130	ARG	2.0
1	D	88	GLU	2.0
1	E	468	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	M	24	GLU	2.0

5.2 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^{th} 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	0.80	0.19	23,24,32,32	0
2	MME	J	1	9/10	0.87	0.21	23,24,32,33	0
2	MME	L	1	9/10	0.88	0.20	23,24,32,32	0
2	MME	M	1	9/10	0.89	0.17	23,23,32,32	0
2	MME	N	1	9/10	0.89	0.16	23,24,32,32	0
2	MME	O	1	9/10	0.89	0.17	23,24,32,33	0
2	MME	P	1	9/10	0.90	0.16	23,24,32,33	0
2	MME	I	1	9/10	0.91	0.16	23,24,32,33	0
1	SMC	G	369	7/8	0.91	0.12	11,12,16,17	0
1	SMC	B	369	7/8	0.92	0.12	11,12,16,16	0
1	SMC	C	369	7/8	0.93	0.10	11,12,17,17	0
1	SMC	A	369	7/8	0.93	0.11	11,12,16,17	0
1	HYP	A	151	8/9	0.94	0.10	8,9,9,9	0
1	SMC	H	369	7/8	0.94	0.09	11,12,16,17	0
1	HYP	D	104	8/9	0.94	0.10	8,8,9,10	0
1	SMC	D	369	7/8	0.94	0.09	11,12,16,17	0
1	HYP	E	104	8/9	0.94	0.07	8,9,9,9	0
1	HYP	F	151	8/9	0.95	0.08	9,9,9,9	0
1	SMC	F	369	7/8	0.95	0.10	11,12,16,17	0
1	HYP	D	151	8/9	0.95	0.10	9,9,9,9	0
1	KCX	E	201	12/13	0.95	0.11	7,9,10,10	0
1	SMC	E	369	7/8	0.95	0.10	11,12,16,17	0
1	HYP	F	104	8/9	0.95	0.10	8,8,9,10	0
1	KCX	G	201	12/13	0.96	0.12	7,9,10,11	0
1	KCX	A	201	12/13	0.96	0.10	8,9,10,11	0
1	HYP	H	151	8/9	0.96	0.09	8,9,9,9	0
1	KCX	H	201	12/13	0.96	0.10	8,9,10,11	0
1	HYP	C	104	8/9	0.96	0.08	8,8,9,10	0
1	HYP	E	151	8/9	0.96	0.10	8,9,9,9	0
1	KCX	C	201	12/13	0.96	0.10	7,9,10,10	0
1	HYP	B	151	8/9	0.96	0.10	8,9,9,9	0
1	KCX	B	201	12/13	0.96	0.11	7,9,10,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SMC	B	256	7/8	0.96	0.09	6,6,7,8	0
1	KCX	D	201	12/13	0.96	0.10	8,9,10,11	0
1	HYP	G	104	8/9	0.96	0.08	8,8,8,9	0
1	HYP	G	151	8/9	0.96	0.08	8,9,9,9	0
1	HYP	H	104	8/9	0.97	0.07	8,8,8,9	0
1	KCX	F	201	12/13	0.97	0.08	8,9,10,11	0
1	HYP	A	104	8/9	0.97	0.07	8,8,9,9	0
1	HYP	C	151	8/9	0.97	0.07	8,9,9,9	0
1	HYP	B	104	8/9	0.98	0.08	8,8,9,9	0
1	SMC	G	256	7/8	0.98	0.06	5,6,7,8	0
1	SMC	D	256	7/8	0.98	0.06	6,6,7,8	0
1	SMC	F	256	7/8	0.98	0.06	6,6,7,9	0
1	SMC	E	256	7/8	0.98	0.07	6,6,7,8	0
1	SMC	A	256	7/8	0.98	0.07	5,5,7,8	0
1	SMC	H	256	7/8	0.98	0.06	5,5,7,8	0
1	SMC	C	256	7/8	0.98	0.07	5,5,7,9	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 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	A	1478	4/4	0.55	0.19	35,36,36,36	0
5	EDO	H	1476	4/4	0.56	0.21	36,37,38,38	0
5	EDO	G	1478	4/4	0.60	0.33	41,43,43,45	0
5	EDO	J	1141	4/4	0.63	0.29	43,43,43,44	0
5	EDO	L	1142	4/4	0.66	0.33	25,25,26,26	4
5	EDO	O	1141	4/4	0.67	0.29	33,33,33,34	0
5	EDO	L	1141	4/4	0.70	0.28	38,38,39,39	1
5	EDO	C	1477	4/4	0.70	0.46	29,29,29,29	4
5	EDO	K	1142	4/4	0.70	0.22	36,37,37,38	0
5	EDO	I	1141	4/4	0.71	0.30	19,20,20,20	4
5	EDO	M	1142	4/4	0.72	0.28	18,18,18,19	4
5	EDO	H	1478	4/4	0.73	0.31	49,50,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	G	1480	4/4	0.74	0.22	41,42,42,42	0
5	EDO	N	1142	4/4	0.74	0.28	28,29,31,32	0
5	EDO	F	1476	4/4	0.74	0.32	17,17,17,18	4
5	EDO	C	1479	4/4	0.75	0.34	46,47,47,47	0
5	EDO	E	1477	4/4	0.75	0.27	50,51,51,52	0
5	EDO	M	1141	4/4	0.75	0.30	22,23,23,24	4
5	EDO	D	1478	4/4	0.76	0.37	22,22,23,24	4
5	EDO	N	1141	4/4	0.77	0.15	40,40,40,40	0
5	EDO	E	1475	4/4	0.78	0.21	31,31,32,32	0
5	EDO	P	1141	4/4	0.78	0.22	36,37,37,37	0
5	EDO	B	1477	4/4	0.80	0.20	51,51,52,52	0
5	EDO	B	1475	4/4	0.82	0.18	17,19,21,21	0
5	EDO	A	1479	4/4	0.83	0.19	37,38,38,39	0
5	EDO	C	1478	4/4	0.83	0.29	26,27,27,27	0
5	EDO	K	1141	4/4	0.84	0.21	33,33,33,34	0
5	EDO	G	1475	4/4	0.85	0.18	19,20,22,22	0
5	EDO	D	1476	4/4	0.86	0.17	38,38,39,39	0
5	EDO	B	1478	4/4	0.86	0.19	30,32,32,32	0
5	EDO	G	1479	4/4	0.87	0.30	8,11,11,13	4
5	EDO	D	1477	4/4	0.87	0.18	21,22,23,24	0
5	EDO	F	1475	4/4	0.88	0.12	23,24,25,25	0
5	EDO	C	1476	4/4	0.89	0.23	12,13,15,15	4
5	EDO	E	1476	4/4	0.90	0.13	25,26,27,27	0
5	EDO	D	1475	4/4	0.90	0.11	21,21,21,22	0
5	EDO	A	1480	4/4	0.91	0.13	26,26,27,27	0
5	EDO	A	1477	4/4	0.94	0.11	19,19,19,20	0
5	EDO	B	1476	4/4	0.94	0.10	18,19,20,20	0
5	EDO	G	1477	4/4	0.94	0.09	25,25,26,27	0
5	EDO	C	1475	4/4	0.94	0.10	19,19,20,21	0
5	EDO	G	1476	4/4	0.95	0.09	20,20,21,22	0
5	EDO	O	1142	4/4	0.95	0.18	24,24,25,25	0
5	EDO	H	1475	4/4	0.95	0.07	19,19,20,20	0
5	EDO	J	1142	4/4	0.96	0.13	23,24,25,26	0
3	CAP	E	477	21/21	0.96	0.09	10,13,15,17	0
5	EDO	H	1477	4/4	0.96	0.09	21,23,23,23	0
3	CAP	F	477	21/21	0.96	0.09	11,13,15,17	0
3	CAP	H	477	21/21	0.96	0.09	9,13,14,17	0
3	CAP	A	476	21/21	0.96	0.10	10,13,14,17	0
3	CAP	G	477	21/21	0.97	0.08	10,13,14,16	0
3	CAP	D	477	21/21	0.97	0.08	10,13,15,17	0
3	CAP	B	477	21/21	0.97	0.08	10,13,14,17	0
3	CAP	C	477	21/21	0.97	0.08	10,13,14,16	0

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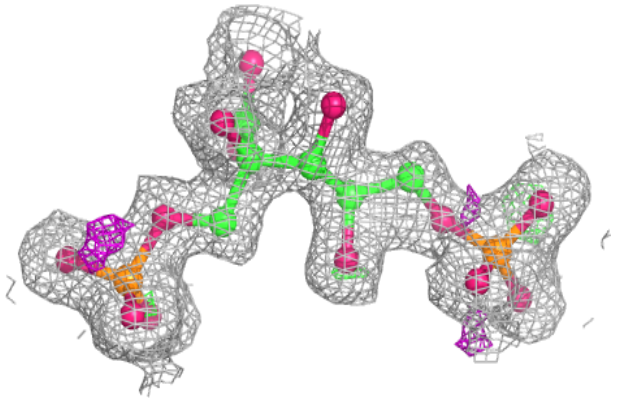
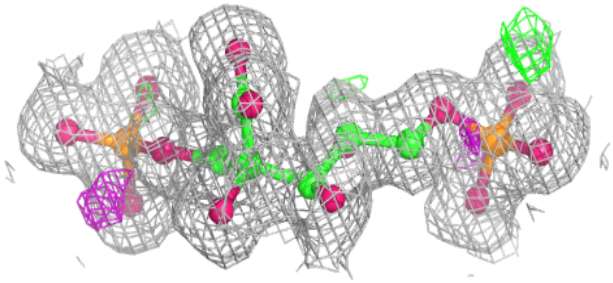
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	476	1/1	0.98	0.05	10,10,10,10	0
4	MG	F	476	1/1	0.98	0.05	10,10,10,10	0
4	MG	G	476	1/1	0.99	0.08	8,8,8,8	0
4	MG	H	476	1/1	0.99	0.04	9,9,9,9	0
4	MG	C	476	1/1	0.99	0.06	9,9,9,9	0
4	MG	D	476	1/1	0.99	0.04	9,9,9,9	0
4	MG	A	477	1/1	0.99	0.04	9,9,9,9	0
4	MG	B	476	1/1	0.99	0.04	9,9,9,9	0

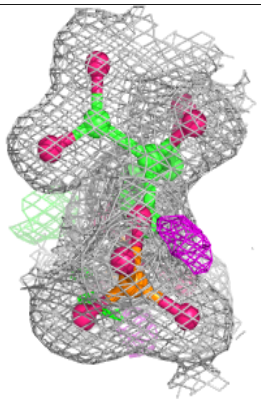
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP 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)

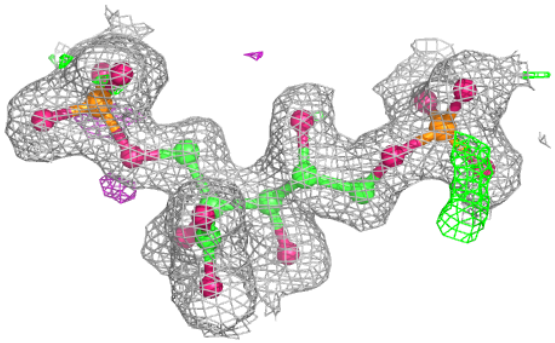


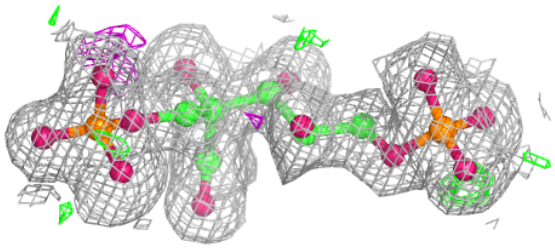


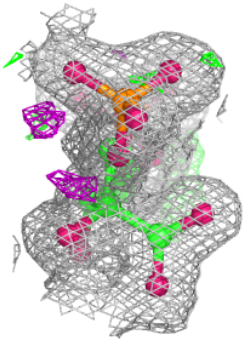


Electron density around CAP A 476:

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

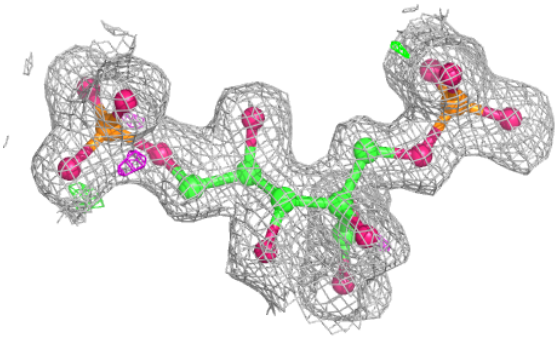


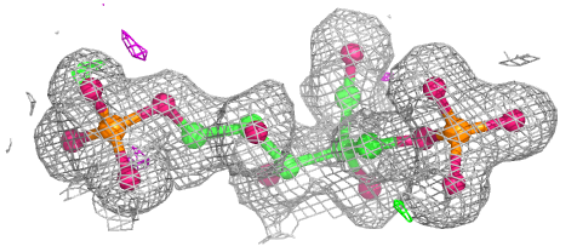


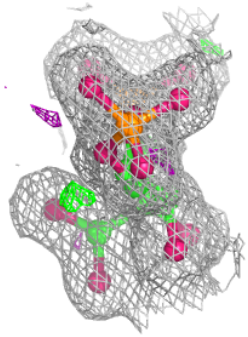


Electron density around CAP G 477:

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

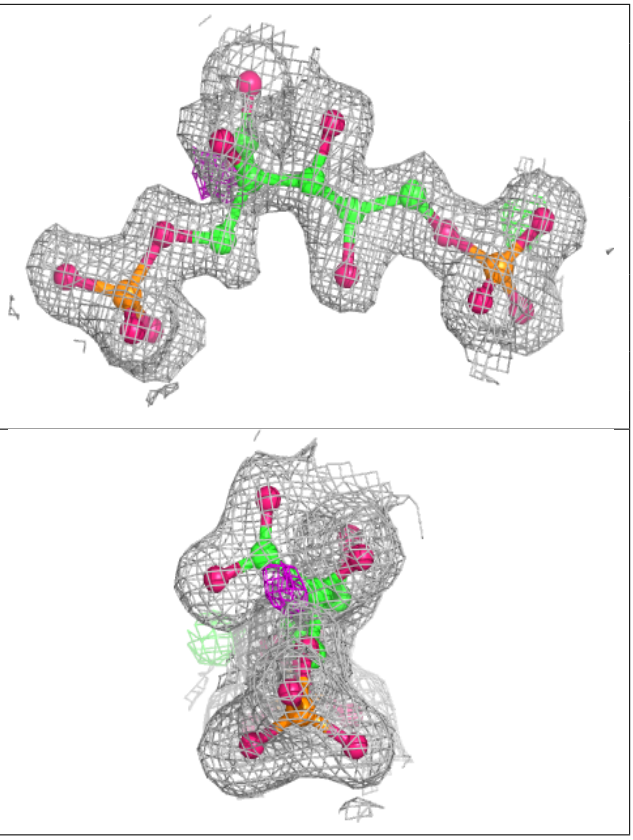


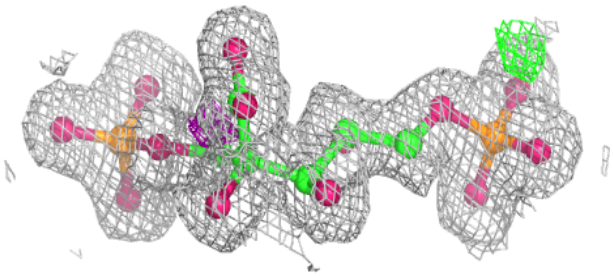




Electron density around CAP D 477:

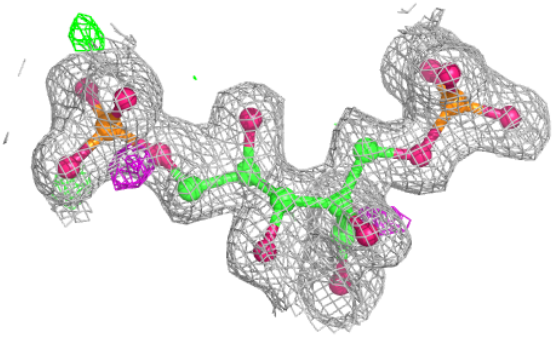
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

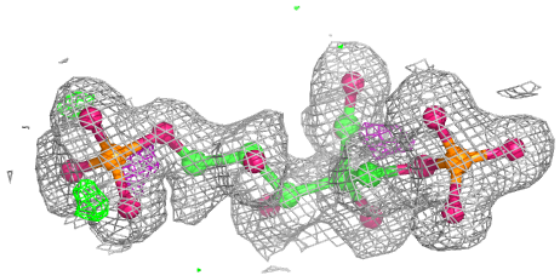


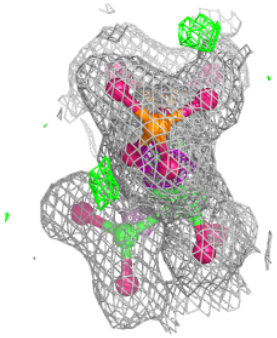


Electron density around CAP B 477:

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

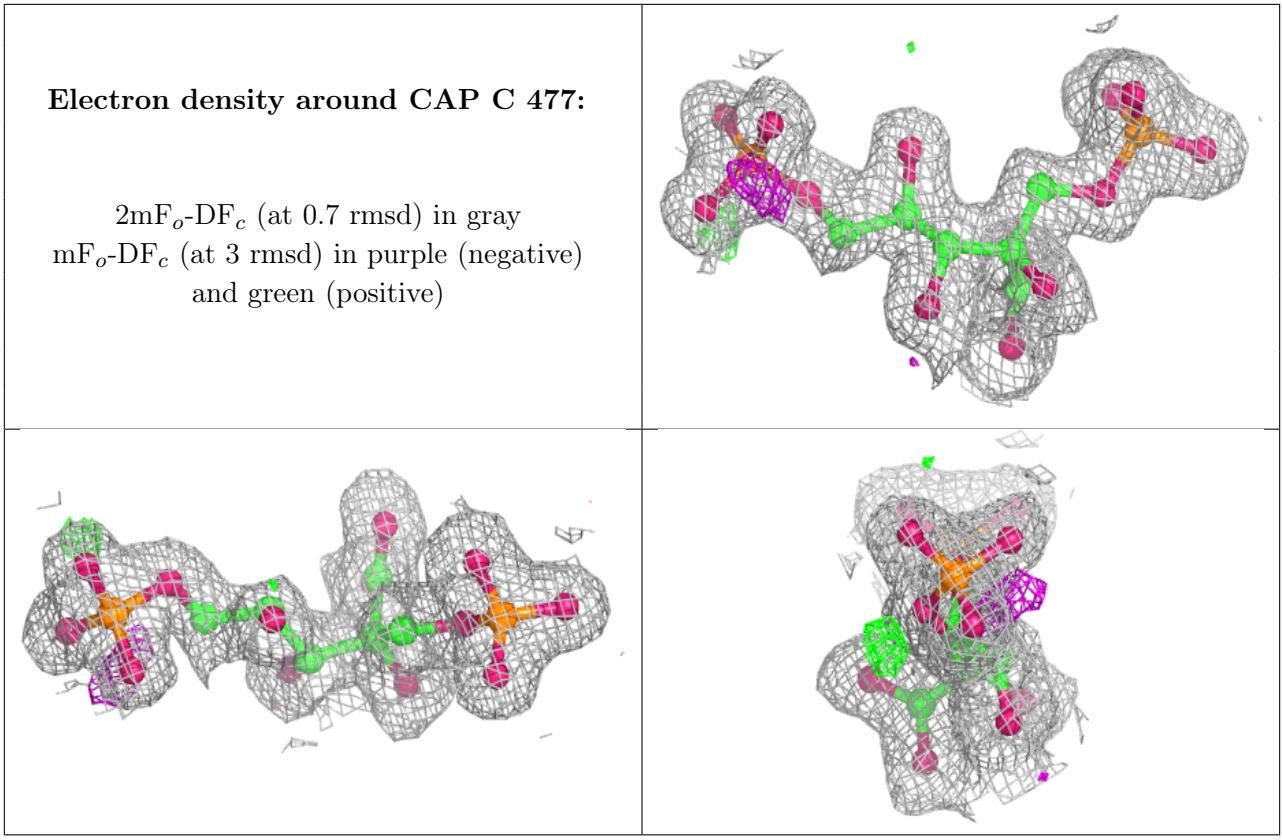






Electron density around CAP C 477:

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



5.5 Other polymers (i)

There are no such residues in this entry.