Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:09 PM BST

PDB ID	:	4LF1
Title	:	Hexameric Form II RuBisCO from Rhodopseudomonas palustris, activated and complexed with 2-CABP
Authors	:	Chan, S.; Satagopan, S.; Sawaya, M.R.; Eisenberg, D.; Tabita, F.R.; Perry, L.J.
Deposited on	:	2013-06-26
Resolution	:	2.38 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 following versions of software and data (see references ⓘ) were used in the production of this report:

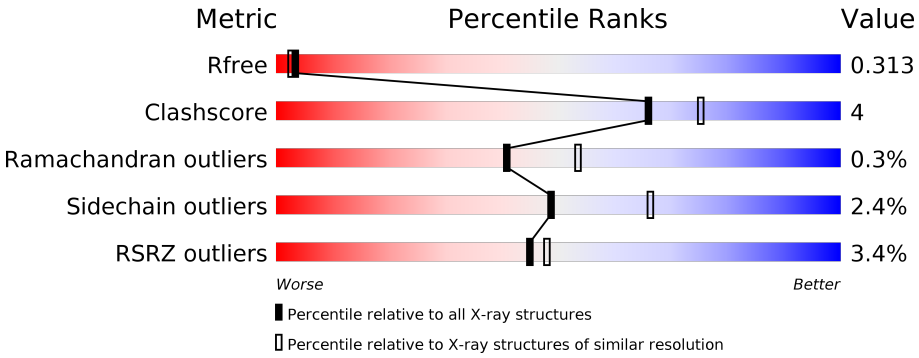
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	481	2% 87% 7% • 5%
1	B	481	3% 88% 5% • 6%
1	C	481	3% 84% 9% • 6%
1	D	481	4% 85% 10% 5%
1	E	481	3% 83% 10% • 5%
1	F	481	4% 85% 8% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21750 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3536	2247	613	657	19			
1	B	453	Total	C	N	O	S	0	0	0
			3505	2226	607	653	19			
1	C	453	Total	C	N	O	S	3	1	0
			3511	2231	608	653	19			
1	D	457	Total	C	N	O	S	0	0	0
			3536	2247	613	657	19			
1	E	455	Total	C	N	O	S	0	1	0
			3525	2239	610	657	19			
1	F	456	Total	C	N	O	S	4	1	0
			3535	2246	614	656	19			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
A	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
A	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
A	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
A	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
B	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
B	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
B	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
B	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
B	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
C	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
C	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
C	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
C	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
C	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
D	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
D	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
D	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
D	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
D	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-19	MET	-	EXPRESSION TAG	UNP Q6N0W9
E	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
E	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
E	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
E	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
E	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9

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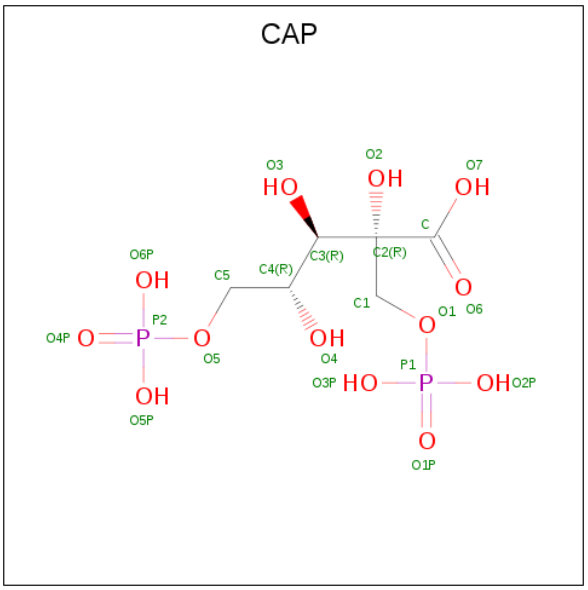
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
F	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
F	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
F	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
F	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	6	13	2		

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

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

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

- Molecule 4 is water.

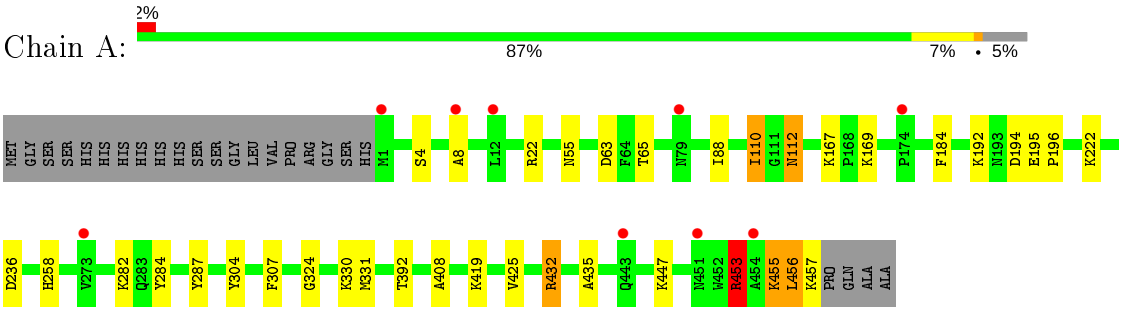
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	79	Total O 79 79	0	0
4	C	75	Total O 75 75	0	0
4	D	70	Total O 70 70	0	0
4	E	79	Total O 79 79	0	0
4	F	89	Total O 89 89	0	0

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.

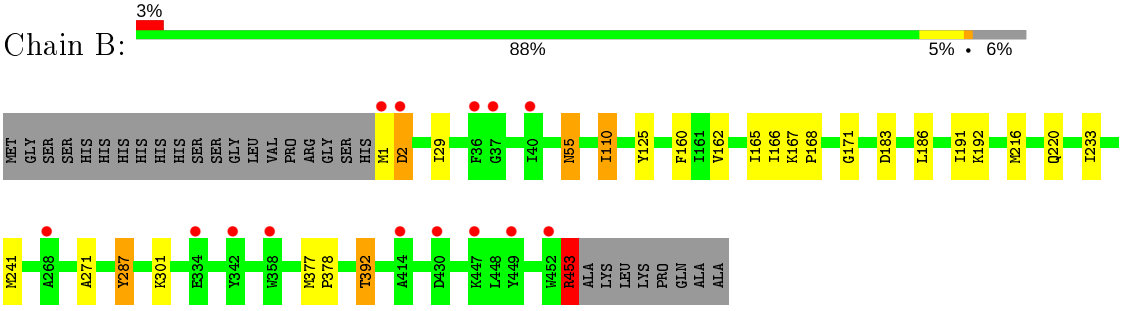
- Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



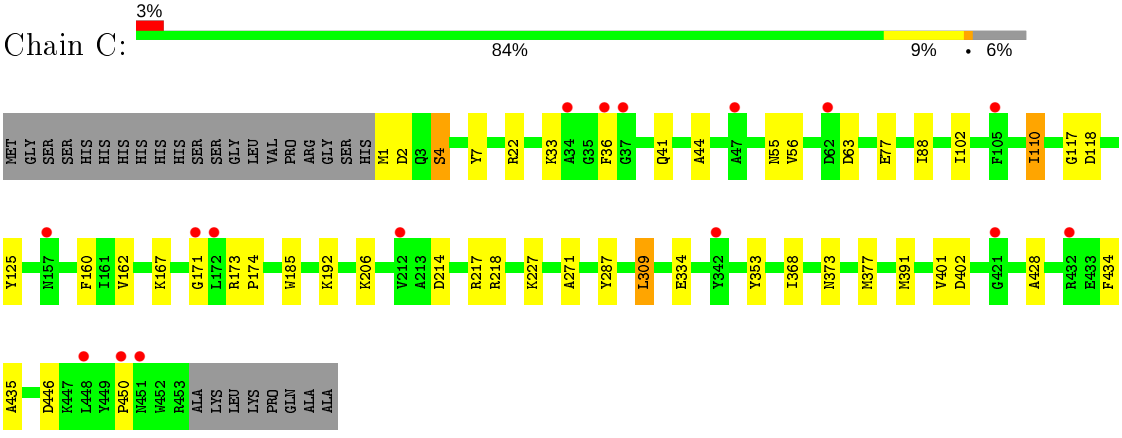
- Molecule 1: Ribulose bisphosphate carboxylase

Chain B:



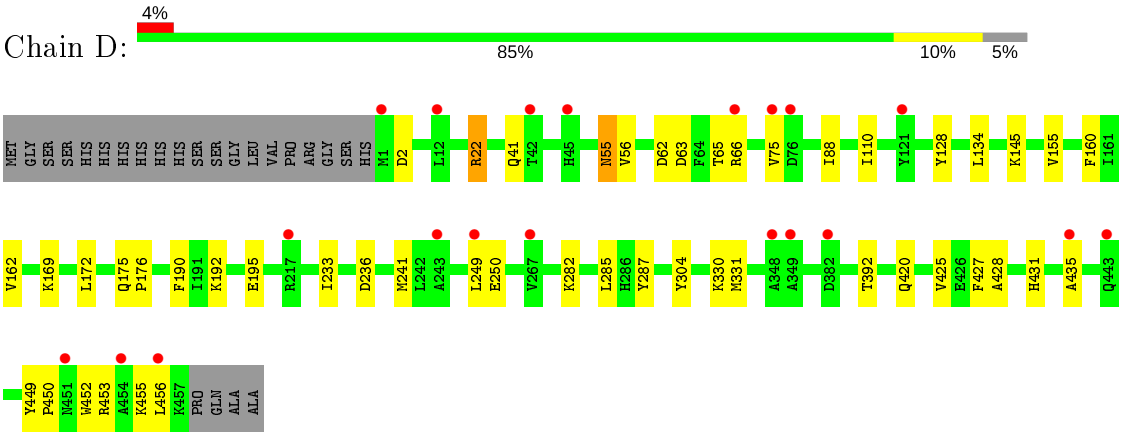
- Molecule 1: Ribulose bisphosphate carboxylase

Chain C:



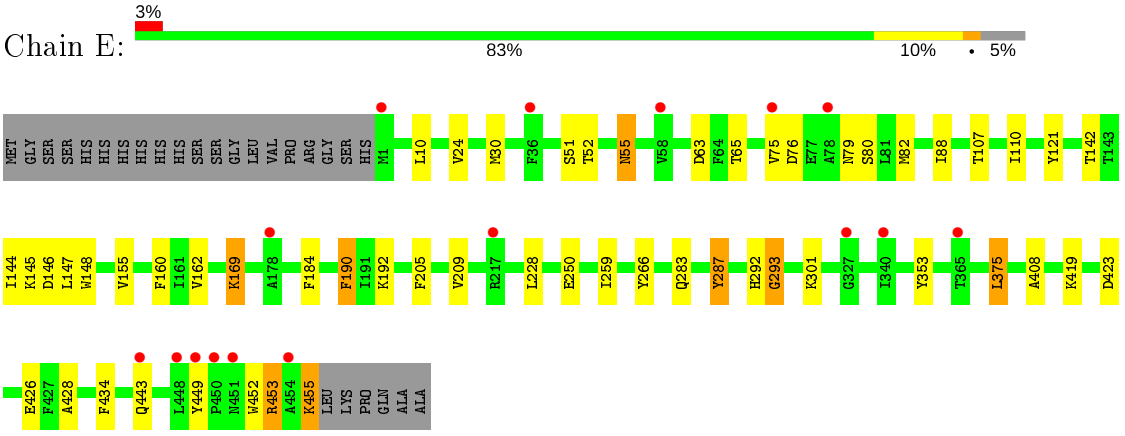
- Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



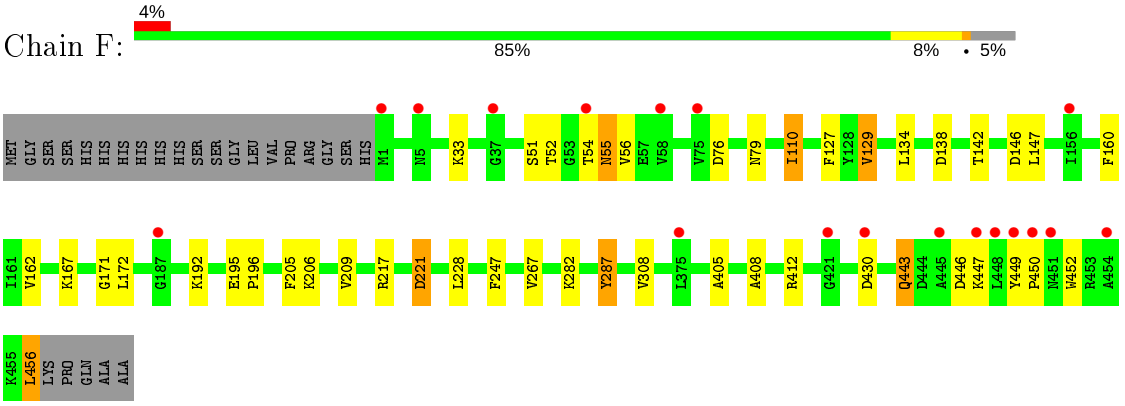
• Molecule 1: Ribulose bisphosphate carboxylase

Chain E:



• Molecule 1: Ribulose bisphosphate carboxylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.03Å 100.72Å 100.69Å 66.51° 108.32° 95.41°	Depositor
Resolution (Å)	71.29 – 2.38 71.18 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (71.29-2.38) 95.8 (71.18-2.36)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.37Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.263 , 0.315 0.263 , 0.313	Depositor DCC
R_{free} test set	5113 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	21750	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	3/3612 (0.1%)	0.77	4/4886 (0.1%)
1	B	0.67	0/3581	0.74	1/4846 (0.0%)
1	C	0.68	0/3590	0.79	6/4857 (0.1%)
1	D	0.67	4/3612 (0.1%)	0.73	1/4886 (0.0%)
1	E	0.75	3/3604 (0.1%)	0.78	0/4876
1	F	0.64	0/3614	0.74	0/4889
All	All	0.68	10/21613 (0.0%)	0.76	12/29240 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	128	TYR	CD2-CE2	-5.85	1.30	1.39
1	E	266	TYR	CD1-CE1	-5.77	1.30	1.39
1	A	304	TYR	CD2-CE2	-5.70	1.30	1.39
1	D	128	TYR	CE2-CZ	-5.41	1.31	1.38
1	E	353	TYR	CD1-CE1	-5.38	1.31	1.39
1	D	128	TYR	CE1-CZ	-5.36	1.31	1.38
1	A	284	TYR	CE1-CZ	-5.21	1.31	1.38
1	E	266	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	284	TYR	CG-CD1	-5.07	1.32	1.39
1	D	128	TYR	CD1-CE1	-5.01	1.31	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	ASP	CB-CG-OD1	7.81	125.33	118.30
1	C	125	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	A	307	PHE	CB-CG-CD1	-6.42	116.30	120.80
1	B	453	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	217	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	453	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	453	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	77	GLU	O-C-N	-5.17	114.43	122.70
1	D	304	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	217	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	217	ARG	CG-CD-NE	-5.01	101.28	111.80

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	3536	0	3414	29	0
1	B	3505	0	3372	19	0
1	C	3511	0	3385	29	0
1	D	3536	0	3414	27	0
1	E	3525	0	3396	39	0
1	F	3535	0	3414	32	0
2	A	21	0	8	0	0
2	B	21	0	9	1	0
2	C	21	0	9	1	0
2	D	21	0	9	0	0
2	E	21	0	9	0	0
2	F	21	0	8	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	78	0	0	1	0
4	B	79	0	0	0	0
4	C	75	0	0	0	0
4	D	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	79	0	0	1	0
4	F	89	0	0	1	0
All	All	21750	0	20447	166	0

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

All (166) 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:E:453:ARG:CB	1:E:453:ARG:HH11	1.45	1.29
1:E:453:ARG:HB2	1:E:453:ARG:NH1	1.52	1.25
1:F:195:GLU:HG2	1:F:196:PRO:HD3	1.41	0.99
1:E:453:ARG:HH11	1:E:453:ARG:HB2	0.76	0.92
1:A:453:ARG:HH21	1:A:453:ARG:HG3	1.38	0.89
1:E:428:ALA:HB2	1:E:434:PHE:HD2	1.45	0.82
1:E:79:ASN:O	1:E:80:SER:HB2	1.80	0.81
1:A:435:ALA:HB1	1:A:456:LEU:HD21	1.63	0.79
1:A:425:VAL:CG1	1:A:455:LYS:HD2	2.12	0.78
1:A:425:VAL:HG11	1:A:455:LYS:HD2	1.64	0.78
1:E:55:ASN:H	1:E:55:ASN:HD22	1.33	0.77
1:F:195:GLU:HG2	1:F:196:PRO:CD	2.15	0.74
1:C:401:VAL:HG13	1:C:402:ASP:OD1	1.90	0.72
1:A:432:ARG:O	1:A:432:ARG:HD3	1.91	0.71
1:C:2:ASP:CG	1:C:41:GLN:HG2	2.11	0.70
1:A:456:LEU:O	1:A:457:LYS:HB2	1.93	0.68
1:E:147:LEU:HD22	1:E:228:LEU:HD13	1.76	0.68
1:E:453:ARG:CB	1:E:453:ARG:NH1	2.31	0.67
1:C:206:LYS:NZ	1:E:250:GLU:OE2	2.23	0.65
1:E:76:ASP:OD2	1:E:79:ASN:ND2	2.30	0.64
1:B:55:ASN:HD22	1:B:55:ASN:H	1.44	0.64
1:C:309:LEU:HD12	1:C:309:LEU:O	1.97	0.64
1:A:195:GLU:HG2	1:A:196:PRO:HD3	1.80	0.63
1:B:1:MET:C	1:B:2:ASP:OD1	2.37	0.62
1:D:2:ASP:OD2	1:D:41:GLN:NE2	2.32	0.62
1:A:456:LEU:O	1:A:457:LYS:CB	2.48	0.61
1:E:428:ALA:HB2	1:E:434:PHE:CD2	2.32	0.60
1:C:309:LEU:HD12	1:C:309:LEU:C	2.23	0.59
1:B:166:ILE:HD11	1:B:191:ILE:HG21	1.83	0.59
1:C:185:TRP:CD1	1:C:227:LYS:HD2	2.38	0.59
1:F:55:ASN:HD22	1:F:55:ASN:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HH21	1:A:453:ARG:CG	2.07	0.58
1:A:432:ARG:C	1:A:432:ARG:HD3	2.24	0.57
1:C:428:ALA:HB2	1:C:434:PHE:HD1	1.70	0.57
1:E:121:TYR:CZ	1:E:301:LYS:HD2	2.40	0.57
1:A:453:ARG:NH2	1:A:453:ARG:HG3	2.16	0.56
1:F:206:LYS:HG2	1:F:247:PHE:CE2	2.40	0.56
1:D:190:PHE:CD1	1:D:190:PHE:C	2.79	0.55
1:D:425:VAL:HG11	1:D:455:LYS:HD2	1.88	0.55
1:F:167:LYS:HE3	2:F:800:CAP:O1P	2.06	0.55
1:A:425:VAL:HG12	1:A:455:LYS:HD2	1.88	0.55
1:D:55:ASN:HD22	1:D:55:ASN:H	1.55	0.54
1:E:51:SER:OG	1:E:52:THR:N	2.40	0.54
1:C:7:TYR:HB2	1:C:44:ALA:HB1	1.90	0.54
1:D:63:ASP:HA	1:D:66:ARG:HD3	1.90	0.53
1:B:183:ASP:HA	1:B:186:LEU:HD12	1.90	0.53
1:D:62:ASP:OD1	1:D:65:THR:OG1	2.24	0.52
1:D:145:LYS:HG3	1:D:155:VAL:HB	1.90	0.52
1:F:142:THR:HG23	1:F:146:ASP:OD2	2.09	0.52
1:B:110:ILE:O	1:B:110:ILE:HG23	2.09	0.52
1:B:55:ASN:HD22	1:B:55:ASN:N	2.03	0.52
1:C:373:ASN:O	1:C:377:MET:HG3	2.10	0.52
1:B:453:ARG:CG	1:B:453:ARG:HH11	2.22	0.52
1:E:30:MET:HB2	1:E:82:MET:HE2	1.90	0.52
1:D:55:ASN:HD22	1:D:55:ASN:N	2.09	0.51
1:A:167:LYS:NZ	1:A:194:ASP:OD2	2.25	0.51
1:C:36:PHE:CD2	1:C:118:ASP:HB3	2.45	0.51
1:D:55:ASN:ND2	1:D:55:ASN:H	2.08	0.51
1:E:144:ILE:HD13	1:E:148:TRP:CZ2	2.46	0.51
1:A:432:ARG:C	1:A:432:ARG:CD	2.79	0.50
1:E:184:PHE:CE1	1:E:408:ALA:HB2	2.46	0.50
1:A:4:SER:O	1:A:8:ALA:HB3	2.12	0.50
1:E:259:ILE:O	1:E:283:GLN:NE2	2.45	0.50
1:A:184:PHE:CD1	1:A:408:ALA:HB2	2.46	0.50
1:E:443:GLN:HB2	4:E:958:HOH:O	2.12	0.50
1:A:453:ARG:NH2	1:A:453:ARG:CG	2.71	0.50
1:A:330:LYS:HE3	1:A:331:MET:CE	2.42	0.49
1:E:184:PHE:CD1	1:E:408:ALA:HB2	2.46	0.49
1:D:425:VAL:CG1	1:D:455:LYS:HD2	2.43	0.49
1:C:368:ILE:HB	1:C:391:MET:HG3	1.94	0.49
1:B:453:ARG:HG2	1:B:453:ARG:HH11	1.77	0.48
1:C:446:ASP:O	1:C:450:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG23	1:A:110:ILE:O	2.13	0.48
1:F:54:THR:HG23	1:F:56:VAL:H	1.77	0.48
1:E:190:PHE:C	1:E:190:PHE:CD1	2.87	0.48
1:C:110:ILE:HG23	1:C:110:ILE:O	2.14	0.48
1:C:167:LYS:HE3	2:C:800:CAP:O1P	2.13	0.48
1:A:112:ASN:ND2	2:B:800:CAP:O6	2.47	0.47
1:B:167:LYS:HA	1:B:168:PRO:C	2.35	0.47
1:B:55:ASN:H	1:B:55:ASN:ND2	2.12	0.47
1:E:169:LYS:HB2	1:E:169:LYS:HE2	1.77	0.47
1:F:172:LEU:HA	1:F:172:LEU:HD23	1.69	0.47
1:A:432:ARG:O	1:A:432:ARG:CD	2.61	0.47
1:D:250:GLU:OE2	1:F:206:LYS:NZ	2.44	0.47
1:E:55:ASN:H	1:E:55:ASN:ND2	2.08	0.47
1:D:160:PHE:CE2	1:D:162:VAL:HG22	2.50	0.46
1:F:449:TYR:O	1:F:452:TRP:HB3	2.15	0.46
1:D:175:GLN:HB3	1:D:176:PRO:HD3	1.97	0.46
1:F:446:ASP:O	1:F:450:PRO:HA	2.16	0.46
1:A:65:THR:HG23	1:B:171:GLY:HA3	1.97	0.46
1:F:160:PHE:CE2	1:F:162:VAL:HG22	2.50	0.46
1:C:428:ALA:HB2	1:C:434:PHE:CD1	2.49	0.46
1:D:22:ARG:HH21	1:D:88:ILE:HD11	1.80	0.46
1:E:142:THR:HG23	1:E:146:ASP:OD2	2.16	0.45
1:A:169:LYS:NZ	1:A:195:GLU:OE2	2.38	0.45
1:A:236:ASP:O	1:B:271:ALA:HA	2.17	0.45
1:C:22:ARG:NH1	1:C:88:ILE:HD11	2.31	0.45
1:C:428:ALA:O	1:C:435:ALA:HB2	2.17	0.45
1:F:129:VAL:HG22	1:F:134:LEU:HB2	1.99	0.45
1:E:455:LYS:HB3	1:E:455:LYS:HE2	1.42	0.45
1:C:160:PHE:CE2	1:C:162:VAL:HG22	2.51	0.45
1:D:169:LYS:NZ	1:D:195:GLU:OE2	2.50	0.45
1:C:271:ALA:HA	1:D:236:ASP:O	2.17	0.45
1:C:1:MET:HE3	1:C:56:VAL:HG23	1.99	0.45
1:E:10:LEU:HD21	1:E:75:VAL:HG22	1.99	0.44
1:F:205:PHE:O	1:F:209:VAL:HG23	2.17	0.44
1:B:233:ILE:O	1:B:241:MET:HG2	2.17	0.44
1:B:216:MET:O	1:B:220:GLN:HG3	2.17	0.44
1:E:423:ASP:HB3	1:E:426:GLU:HB2	1.98	0.44
1:A:195:GLU:CG	1:A:196:PRO:HD3	2.45	0.44
1:A:324:GLY:HA2	4:A:954:HOH:O	2.18	0.44
1:F:127:PHE:CE1	1:F:308:VAL:HG13	2.51	0.44
1:E:145:LYS:HG3	1:E:155:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:OD1	1:C:4:SER:OG	2.34	0.44
1:E:419:LYS:HB2	1:E:419:LYS:HE3	1.78	0.43
1:C:214:ASP:O	1:C:218:ARG:HG3	2.17	0.43
1:A:22:ARG:NH1	1:A:88:ILE:HD11	2.33	0.43
1:B:165:ILE:HD11	1:B:392:THR:HB	2.00	0.43
1:E:24:VAL:HG23	1:E:88:ILE:HG22	2.00	0.43
1:E:292:HIS:CG	1:E:293:GLY:N	2.86	0.43
1:A:282:LYS:HE3	1:F:138:ASP:HA	1.99	0.43
1:A:330:LYS:HE3	1:A:331:MET:HE1	1.99	0.43
1:D:55:ASN:ND2	1:D:55:ASN:N	2.65	0.43
1:E:287:TYR:C	1:E:287:TYR:CD1	2.92	0.43
1:E:107:THR:OG1	1:F:267:VAL:HG21	2.18	0.43
1:F:206:LYS:HG2	1:F:247:PHE:CZ	2.54	0.43
1:B:160:PHE:CE2	1:B:162:VAL:HG22	2.53	0.43
1:C:33:LYS:HD2	1:C:117:GLY:O	2.19	0.42
1:E:65:THR:HG23	1:F:171:GLY:HA3	2.02	0.42
1:B:377:MET:N	1:B:378:PRO:CD	2.83	0.42
1:C:1:MET:CE	1:C:56:VAL:HG23	2.49	0.42
1:D:452:TRP:CE3	1:D:453:ARG:HA	2.55	0.42
1:F:456:LEU:HD13	1:F:456:LEU:N	2.34	0.42
1:D:233:ILE:O	1:D:241:MET:HG2	2.19	0.42
1:C:171:GLY:HA3	1:D:65:THR:HG23	2.00	0.42
1:D:134:LEU:HD12	1:D:134:LEU:O	2.20	0.42
1:E:160:PHE:CE2	1:E:162:VAL:HG22	2.55	0.42
1:D:172:LEU:HD22	1:D:176:PRO:HB2	2.03	0.41
1:E:375:LEU:HB3	1:E:449:TYR:HE2	1.85	0.41
1:C:102:ILE:HD12	1:C:102:ILE:HA	1.97	0.41
1:F:134:LEU:O	1:F:134:LEU:HD12	2.21	0.41
1:F:55:ASN:HD22	1:F:55:ASN:N	2.15	0.41
1:F:76:ASP:OD2	1:F:79:ASN:ND2	2.54	0.41
1:C:173:ARG:HB3	1:C:174:PRO:HD2	2.02	0.41
1:D:428:ALA:O	1:D:435:ALA:HB2	2.20	0.41
1:E:287:TYR:HD1	1:E:287:TYR:C	2.23	0.41
1:E:79:ASN:O	1:E:80:SER:CB	2.50	0.41
1:F:443:GLN:O	1:F:447:LYS:HG3	2.20	0.41
1:D:449:TYR:O	1:D:452:TRP:HD1	2.03	0.41
1:F:110:ILE:O	1:F:110:ILE:HG23	2.21	0.41
1:F:147:LEU:HD22	1:F:228:LEU:HD13	2.03	0.41
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.87	0.41
1:D:330:LYS:HE3	1:D:331:MET:CE	2.50	0.41
1:C:2:ASP:OD1	1:C:41:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:SER:OG	1:F:52:THR:N	2.53	0.41
1:C:428:ALA:HB1	1:C:435:ALA:HA	2.03	0.40
1:F:412:ARG:HD3	4:F:943:HOH:O	2.21	0.40
1:E:205:PHE:O	1:E:209:VAL:HG23	2.20	0.40
1:E:452:TRP:CD2	1:E:453:ARG:N	2.89	0.40
1:B:287:TYR:CD1	1:B:287:TYR:C	2.95	0.40
1:D:427:PHE:CE1	1:D:431:HIS:CE1	3.09	0.40
1:B:29:ILE:HG13	1:B:125:TYR:CE1	2.56	0.40
1:F:287:TYR:CD1	1:F:287:TYR:C	2.94	0.40
1:F:405:ALA:O	1:F:408:ALA:HB3	2.20	0.40
1:F:195:GLU:CG	1:F:196:PRO:HD3	2.31	0.40

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	454/481 (94%)	435 (96%)	17 (4%)	2 (0%)	34	46
1	B	450/481 (94%)	430 (96%)	19 (4%)	1 (0%)	47	61
1	C	451/481 (94%)	430 (95%)	20 (4%)	1 (0%)	47	61
1	D	454/481 (94%)	436 (96%)	16 (4%)	2 (0%)	34	46
1	E	453/481 (94%)	437 (96%)	14 (3%)	2 (0%)	34	46
1	F	454/481 (94%)	438 (96%)	15 (3%)	1 (0%)	47	61
All	All	2716/2886 (94%)	2606 (96%)	101 (4%)	9 (0%)	41	53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	293	GLY

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	110	ILE
1	E	110	ILE
1	C	110	ILE
1	F	110	ILE
1	D	110	ILE
1	B	110	ILE
1	D	450	PRO

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	353/372 (95%)	342 (97%)	11 (3%)	40	57
1	B	350/372 (94%)	344 (98%)	6 (2%)	60	76
1	C	351/372 (94%)	345 (98%)	6 (2%)	60	76
1	D	353/372 (95%)	343 (97%)	10 (3%)	43	61
1	E	352/372 (95%)	344 (98%)	8 (2%)	50	68
1	F	353/372 (95%)	342 (97%)	11 (3%)	40	57
All	All	2112/2232 (95%)	2060 (98%)	52 (2%)	49	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	222	LYS
1	A	258	HIS
1	A	287	TYR
1	A	392	THR
1	A	419	LYS
1	A	432	ARG
1	A	447	LYS
1	A	453	ARG
1	A	455	LYS

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Mol	Chain	Res	Type
1	A	456	LEU
1	B	2	ASP
1	B	55	ASN
1	B	287	TYR
1	B	301	LYS
1	B	392	THR
1	B	453	ARG
1	C	4	SER
1	C	55	ASN
1	C	63	ASP
1	C	287	TYR
1	C	309	LEU
1	C	334	GLU
1	D	22	ARG
1	D	55	ASN
1	D	56	VAL
1	D	75	VAL
1	D	282	LYS
1	D	285	LEU
1	D	287	TYR
1	D	392	THR
1	D	420	GLN
1	D	456	LEU
1	E	55	ASN
1	E	63	ASP
1	E	169	LYS
1	E	190	PHE
1	E	287	TYR
1	E	375	LEU
1	E	453	ARG
1	E	455	LYS
1	F	33	LYS
1	F	55	ASN
1	F	129	VAL
1	F	217[A]	ARG
1	F	217[B]	ARG
1	F	221	ASP
1	F	282	LYS
1	F	287	TYR
1	F	430	ASP
1	F	443	GLN
1	F	456	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	79	ASN
1	B	55	ASN
1	C	55	ASN
1	C	79	ASN
1	D	55	ASN
1	D	420	GLN
1	E	55	ASN
1	F	55	ASN
1	F	451	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	C	192	1,3	7,11,12	1.32	1 (14%)	4,12,14	0.88	0
1	KCX	A	192	1,3	7,11,12	1.06	1 (14%)	4,12,14	0.88	0
1	KCX	E	192	1,3	7,11,12	1.27	1 (14%)	4,12,14	0.83	0
1	KCX	B	192	1,3	7,11,12	1.37	1 (14%)	4,12,14	0.59	0
1	KCX	D	192	1,3	7,11,12	1.26	1 (14%)	4,12,14	0.97	0
1	KCX	F	192	1,3	7,11,12	1.29	1 (14%)	4,12,14	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	192	1,3	-	0/7/10/12	-
1	KCX	A	192	1,3	-	0/7/10/12	-
1	KCX	E	192	1,3	-	0/7/10/12	-
1	KCX	B	192	1,3	-	0/7/10/12	-
1	KCX	D	192	1,3	-	0/7/10/12	-
1	KCX	F	192	1,3	-	0/7/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	KCX	CE-NZ	3.15	1.52	1.45
1	F	192	KCX	CE-NZ	3.05	1.52	1.45
1	E	192	KCX	CE-NZ	2.97	1.52	1.45
1	C	192	KCX	CE-NZ	2.84	1.51	1.45
1	D	192	KCX	CE-NZ	2.70	1.51	1.45
1	A	192	KCX	CE-NZ	2.34	1.50	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CAP	B	800	3	15,20,20	0.89	0	20,31,31	1.05	1 (5%)
2	CAP	F	800	3	15,20,20	0.94	0	20,31,31	0.97	0
2	CAP	D	800	3	15,20,20	0.84	0	20,31,31	0.83	0
2	CAP	A	800	3	15,20,20	0.88	0	20,31,31	1.08	2 (10%)
2	CAP	E	800	3	15,20,20	0.83	0	20,31,31	0.98	1 (5%)
2	CAP	C	800	3	15,20,20	0.74	0	20,31,31	1.23	4 (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	CAP	B	800	3	-	4/23/29/29	-
2	CAP	F	800	3	-	4/23/29/29	-
2	CAP	D	800	3	-	3/23/29/29	-
2	CAP	A	800	3	-	2/23/29/29	-
2	CAP	E	800	3	-	3/23/29/29	-
2	CAP	C	800	3	-	10/23/29/29	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	CAP	O1-P1-O1P	3.30	115.74	106.47
2	E	800	CAP	O5P-P2-O5	3.06	114.87	106.73
2	A	800	CAP	O5P-P2-O5	2.58	113.59	106.73
2	A	800	CAP	O3P-P1-O1	2.41	113.15	106.73
2	C	800	CAP	P1-O1-C1	2.33	124.70	118.30
2	C	800	CAP	O5P-P2-O5	2.28	112.79	106.73
2	C	800	CAP	O1-P1-O1P	2.14	112.49	106.47
2	C	800	CAP	O3P-P1-O1	2.05	112.18	106.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	CAP	O3-C3-C4-O4
2	F	800	CAP	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
2	D	800	CAP	O4-C4-C5-O5
2	C	800	CAP	O1-C1-C2-C
2	C	800	CAP	O1-C1-C2-O2
2	C	800	CAP	C2-C3-C4-O4
2	C	800	CAP	O3-C3-C4-O4
2	C	800	CAP	C1-O1-P1-O1P
2	C	800	CAP	C1-O1-P1-O2P
2	C	800	CAP	C1-O1-P1-O3P
2	B	800	CAP	O2-C2-C3-C4
2	F	800	CAP	O2-C2-C3-C4
2	D	800	CAP	O2-C2-C3-C4
2	A	800	CAP	O2-C2-C3-C4
2	E	800	CAP	O2-C2-C3-C4
2	C	800	CAP	O2-C2-C3-C4
2	F	800	CAP	C3-C4-C5-O5
2	D	800	CAP	C3-C4-C5-O5
2	C	800	CAP	C-C2-C3-C4
2	C	800	CAP	O1-C1-C2-C3
2	E	800	CAP	C4-C5-O5-P2
2	E	800	CAP	O3-C3-C4-O4
2	B	800	CAP	O4-C4-C5-O5
2	A	800	CAP	O4-C4-C5-O5
2	B	800	CAP	C2-C3-C4-O4
2	F	800	CAP	O1-C1-C2-O2

There are no ring outliers.

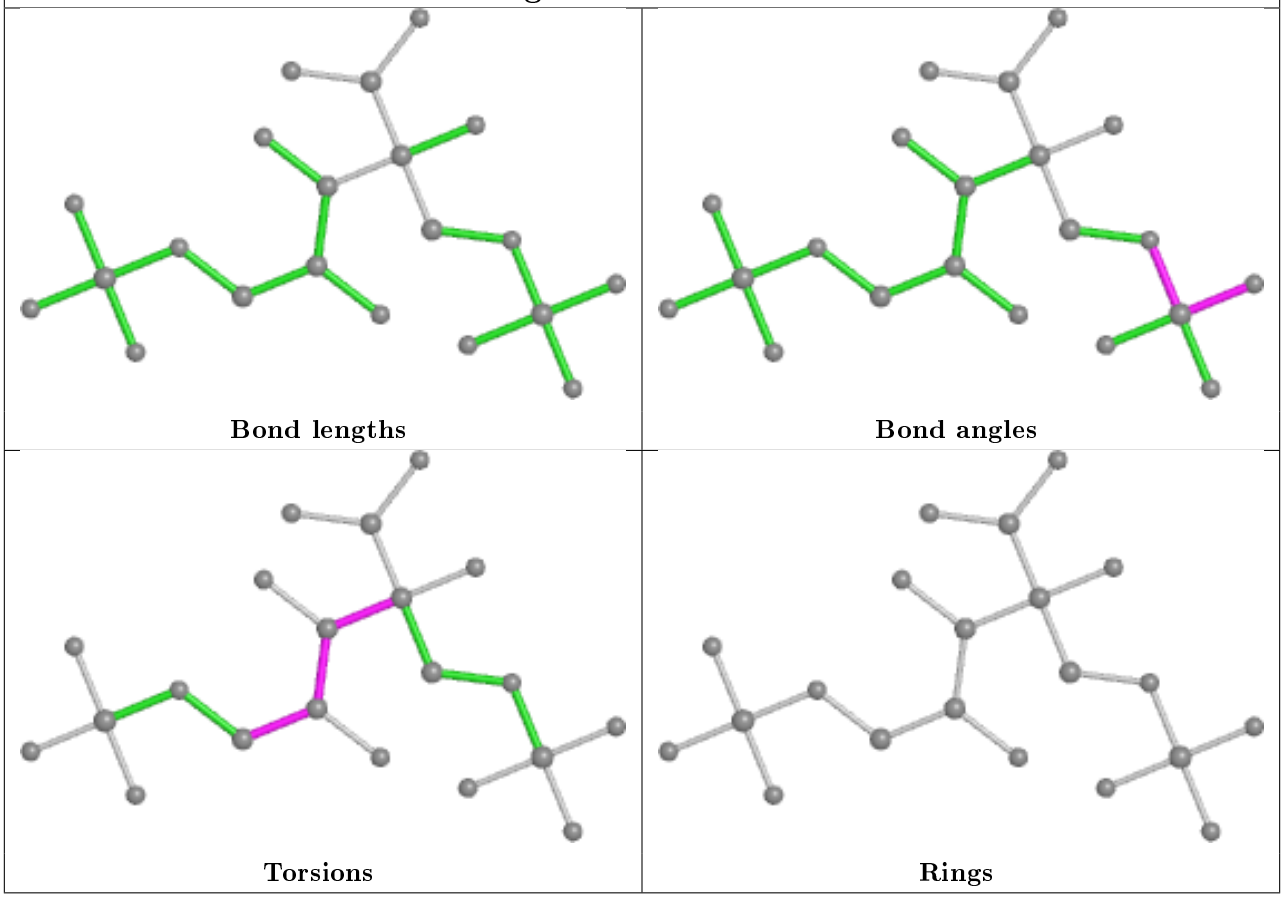
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	CAP	1	0
2	F	800	CAP	1	0
2	C	800	CAP	1	0

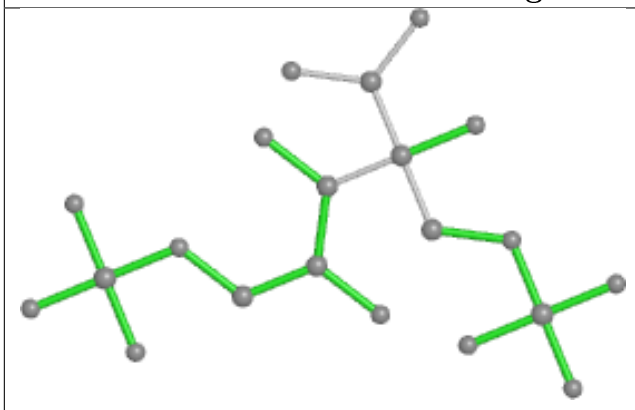
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

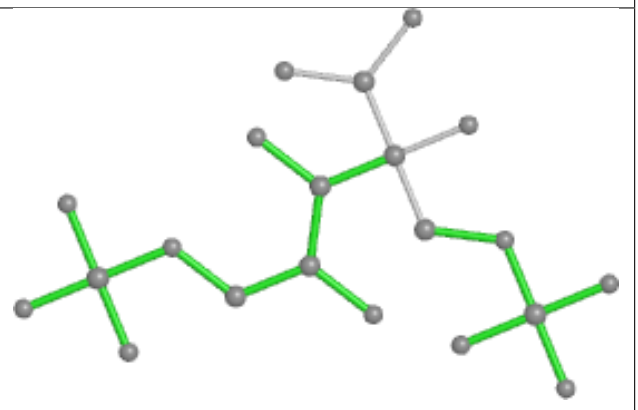
Ligand CAP B 800



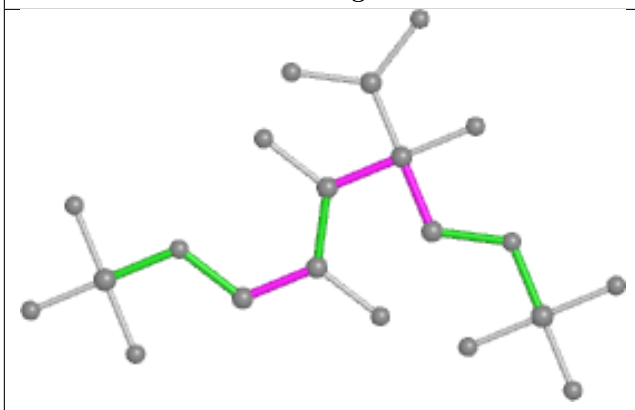
Ligand CAP F 800



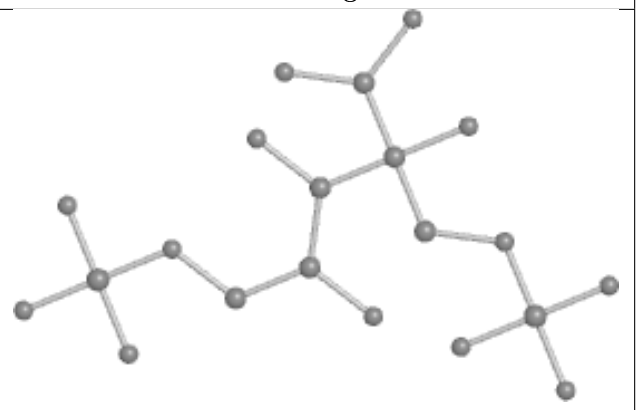
Bond lengths



Bond angles

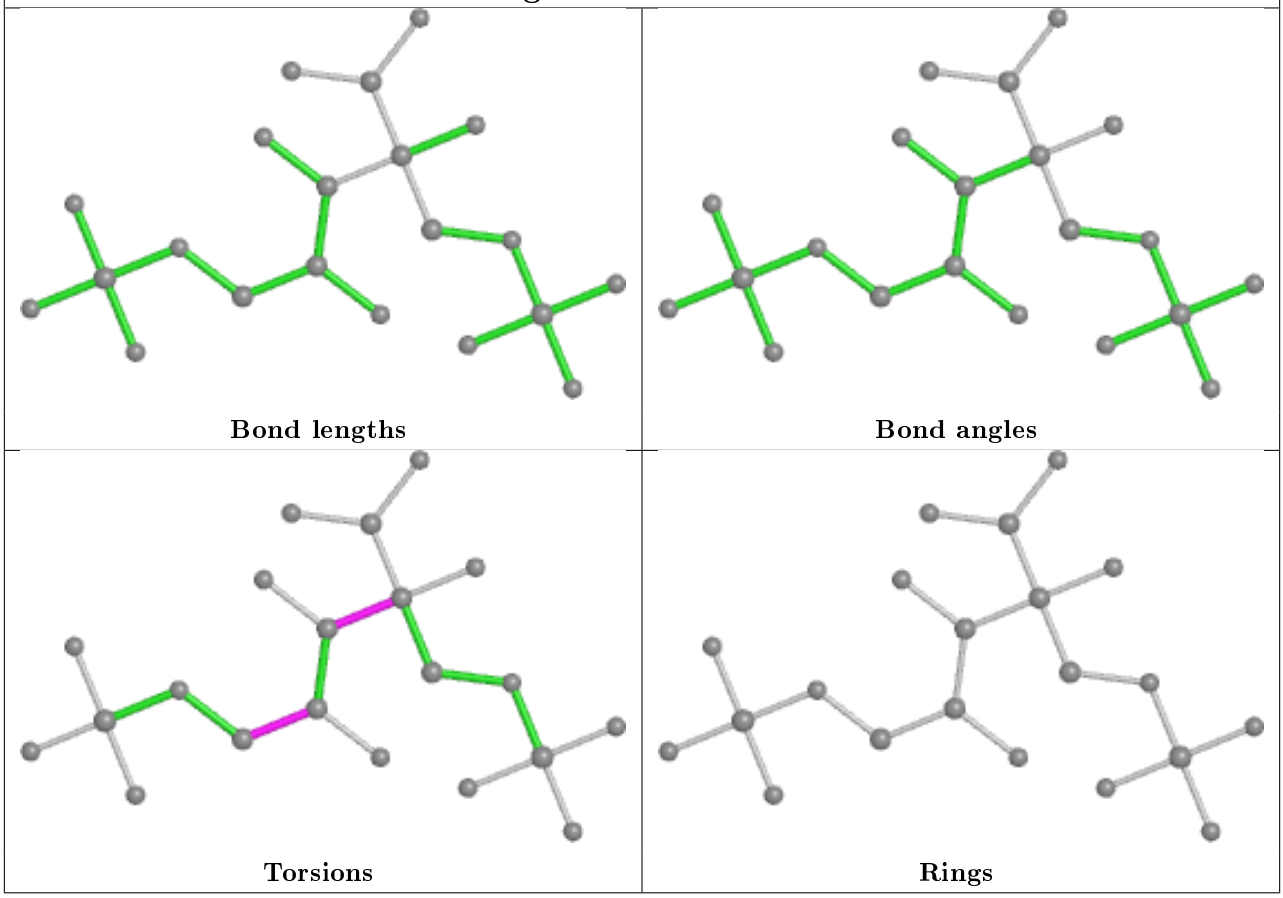


Torsions

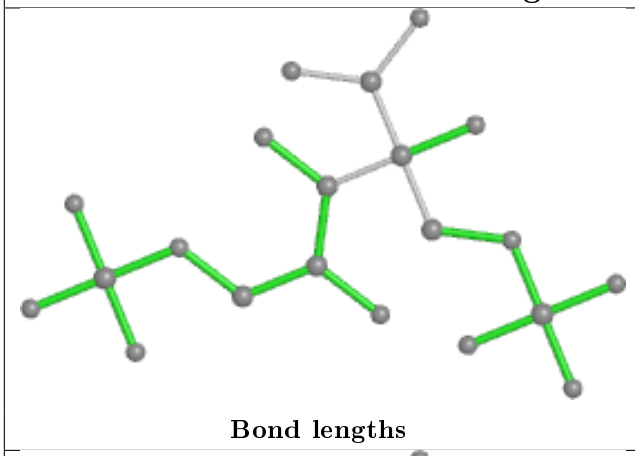


Rings

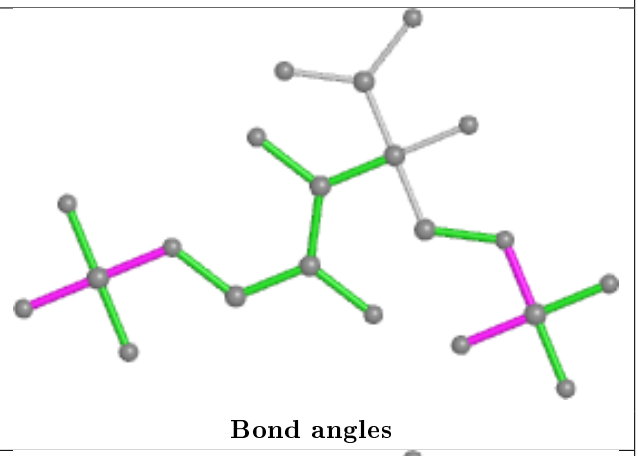
Ligand CAP D 800



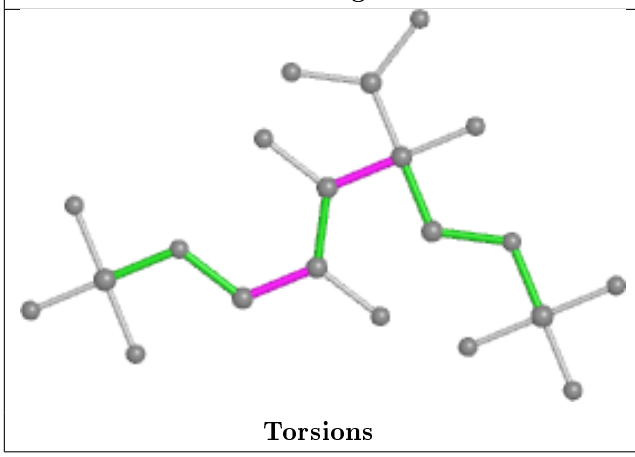
Ligand CAP A 800



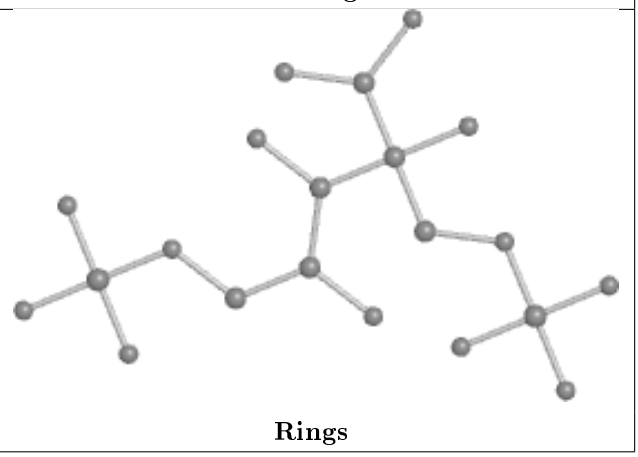
Bond lengths



Bond angles

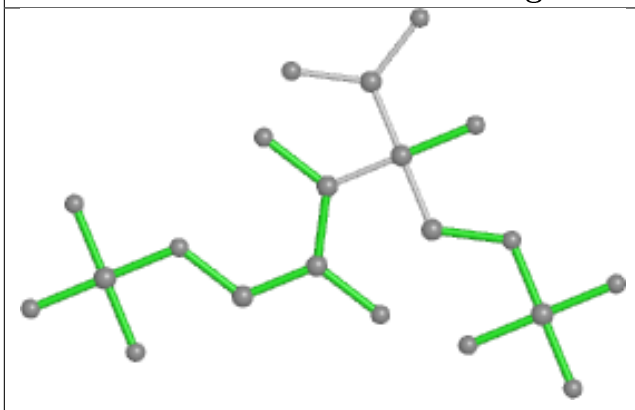


Torsions

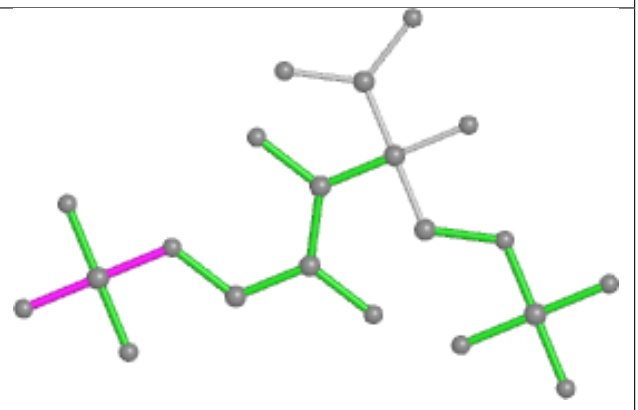


Rings

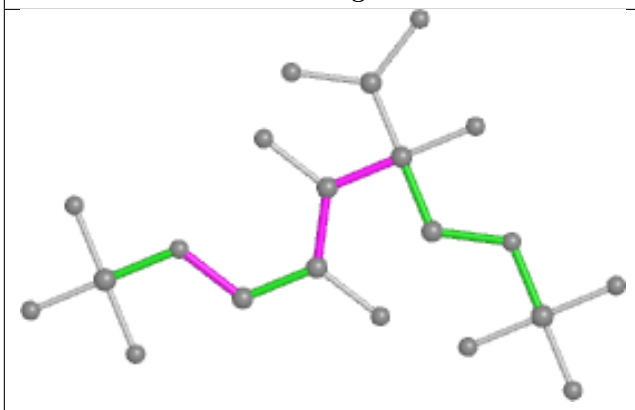
Ligand CAP E 800



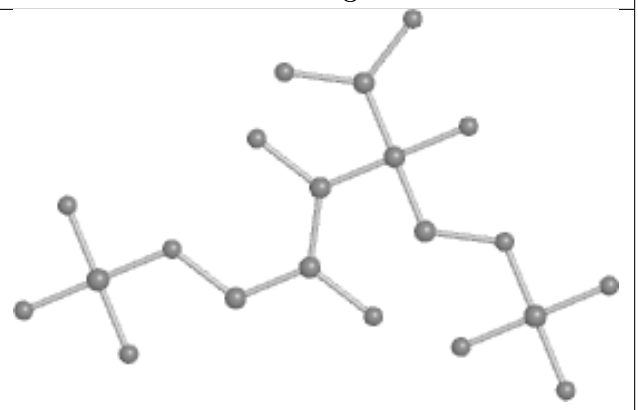
Bond lengths



Bond angles

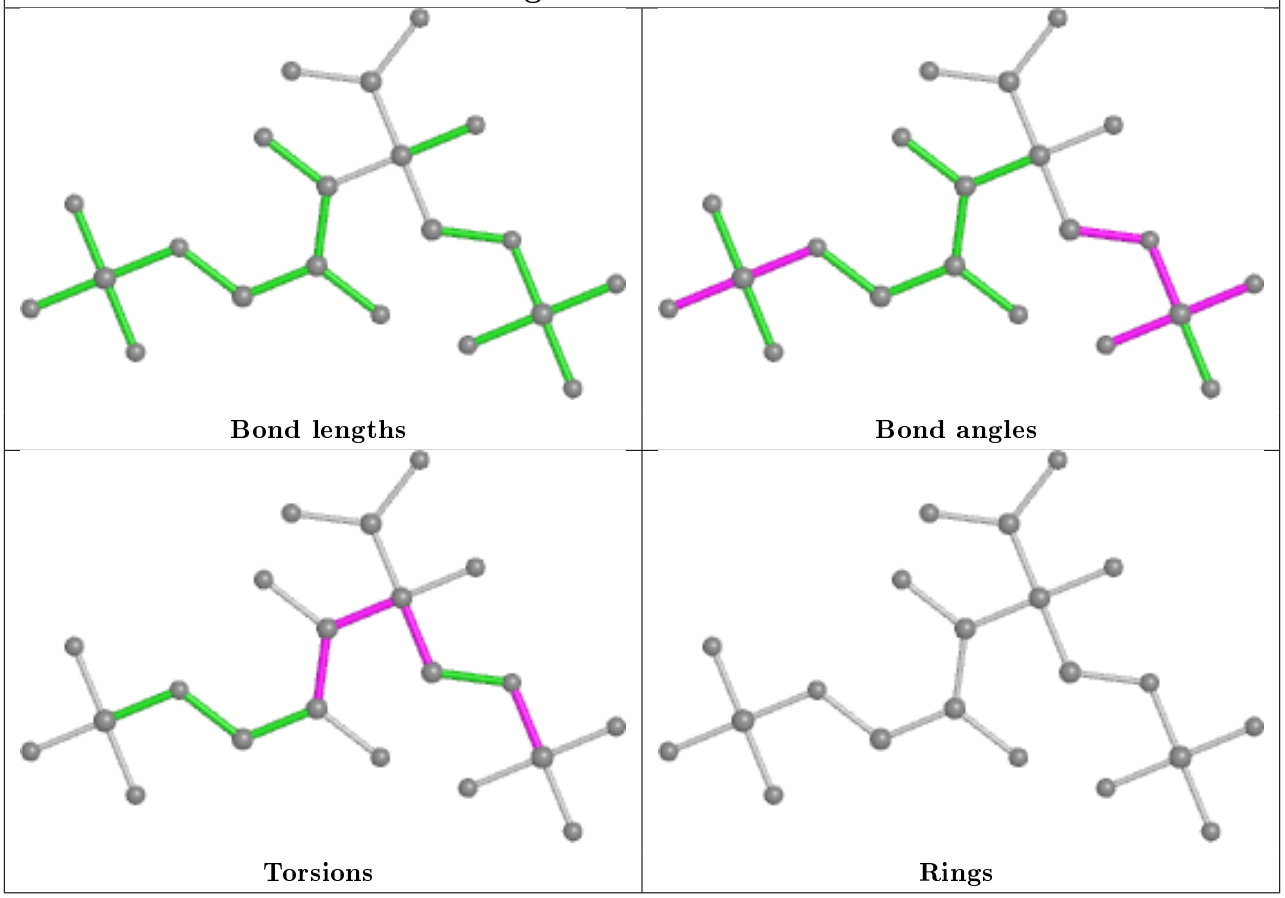


Torsions



Rings

Ligand CAP C 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	456/481 (94%)	0.56	9 (1%)	65	66	5, 13, 26, 54	0
1	B	452/481 (93%)	0.54	14 (3%)	49	51	5, 13, 26, 49	0
1	C	452/481 (93%)	0.50	16 (3%)	44	47	6, 13, 29, 49	1 (0%)
1	D	456/481 (94%)	0.58	20 (4%)	34	37	4, 13, 26, 74	3 (0%)
1	E	454/481 (94%)	0.60	16 (3%)	44	47	6, 13, 27, 47	0
1	F	455/481 (94%)	0.62	18 (3%)	38	41	8, 13, 27, 54	1 (0%)
All	All	2725/2886 (94%)	0.57	93 (3%)	45	48	4, 13, 27, 74	5 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.1
1	D	454	ALA	4.6
1	E	451	ASN	4.6
1	F	450	PRO	4.0
1	D	456	LEU	3.9
1	F	448	LEU	3.8
1	F	1	MET	3.5
1	A	454	ALA	3.5
1	C	34	ALA	3.4
1	F	156	ILE	3.3
1	B	414	ALA	3.3
1	C	450	PRO	3.3
1	A	12	LEU	3.3
1	E	217	ARG	3.2
1	B	430	ASP	3.2
1	D	382	ASP	3.2
1	B	2	ASP	3.1
1	E	449	TYR	3.0
1	D	75	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	75	VAL	2.9
1	C	432	ARG	2.8
1	D	12	LEU	2.8
1	A	1	MET	2.8
1	A	443	GLN	2.8
1	F	430	ASP	2.8
1	F	447	LYS	2.8
1	E	178	ALA	2.7
1	F	37	GLY	2.7
1	C	62	ASP	2.7
1	E	1	MET	2.7
1	E	448	LEU	2.7
1	F	454	ALA	2.7
1	C	448	LEU	2.6
1	F	75	VAL	2.6
1	B	36	PHE	2.5
1	C	171	GLY	2.5
1	E	365	THR	2.5
1	A	451	ASN	2.5
1	D	435	ALA	2.5
1	F	187	GLY	2.5
1	B	358	TRP	2.5
1	D	243	ALA	2.5
1	B	268	ALA	2.4
1	B	342	TYR	2.4
1	D	45	HIS	2.4
1	C	342	TYR	2.4
1	F	449	TYR	2.4
1	F	375	LEU	2.4
1	E	450	PRO	2.3
1	C	47	ALA	2.3
1	B	37	GLY	2.3
1	D	217	ARG	2.3
1	F	451	ASN	2.3
1	C	37	GLY	2.3
1	C	105	PHE	2.3
1	E	78	ALA	2.3
1	E	454	ALA	2.3
1	D	349	ALA	2.3
1	C	421	GLY	2.2
1	E	340	ILE	2.2
1	F	54	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	451	ASN	2.2
1	D	267	VAL	2.2
1	A	8	ALA	2.2
1	C	451	ASN	2.2
1	C	157	ASN	2.1
1	E	36	PHE	2.1
1	A	174	PRO	2.1
1	B	452	TRP	2.1
1	D	66	ARG	2.1
1	E	58	VAL	2.1
1	C	36	PHE	2.1
1	D	42	THR	2.1
1	D	348	ALA	2.1
1	F	421	GLY	2.1
1	F	58	VAL	2.1
1	D	76	ASP	2.1
1	D	121	TYR	2.1
1	C	172	LEU	2.1
1	D	249	LEU	2.1
1	B	1	MET	2.1
1	A	79	ASN	2.1
1	C	212	VAL	2.1
1	B	40	ILE	2.1
1	D	443	GLN	2.1
1	F	5	ASN	2.1
1	E	327	GLY	2.1
1	B	334	GLU	2.0
1	B	449	TYR	2.0
1	E	443	GLN	2.0
1	F	445	ALA	2.0
1	A	273	VAL	2.0
1	B	447	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
1	KCX	A	192	12/13	0.84	0.19	9,11,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	F	192	12/13	0.84	0.14	9,11,22,25	0
1	KCX	D	192	12/13	0.85	0.19	9,11,22,25	0
1	KCX	C	192	12/13	0.87	0.17	9,10,22,25	0
1	KCX	B	192	12/13	0.89	0.14	9,11,22,25	0
1	KCX	E	192	12/13	0.91	0.15	9,11,22,25	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

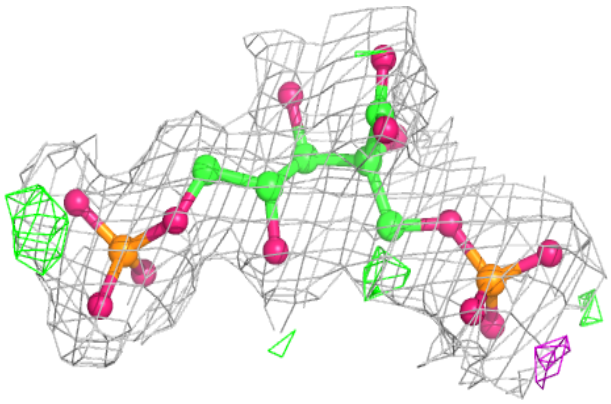
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

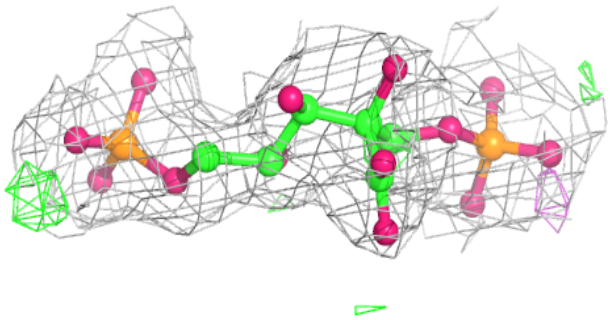
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	801	1/1	0.87	0.09	33,33,33,33	0
3	MG	F	801	1/1	0.89	0.09	11,11,11,11	0
3	MG	D	801	1/1	0.90	0.06	13,13,13,13	0
3	MG	C	801	1/1	0.90	0.11	33,33,33,33	0
2	CAP	F	800	21/21	0.92	0.12	4,16,26,29	0
2	CAP	B	800	21/21	0.94	0.12	2,10,16,22	0
2	CAP	E	800	21/21	0.94	0.12	2,13,19,26	0
3	MG	E	801	1/1	0.94	0.07	21,21,21,21	0
2	CAP	C	800	21/21	0.95	0.12	2,12,18,24	0
2	CAP	A	800	21/21	0.96	0.11	2,12,20,26	0
2	CAP	D	800	21/21	0.96	0.10	4,15,24,34	0
3	MG	A	801	1/1	0.97	0.06	12,12,12,12	0

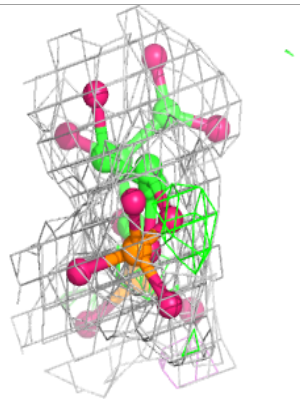
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP F 800:

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

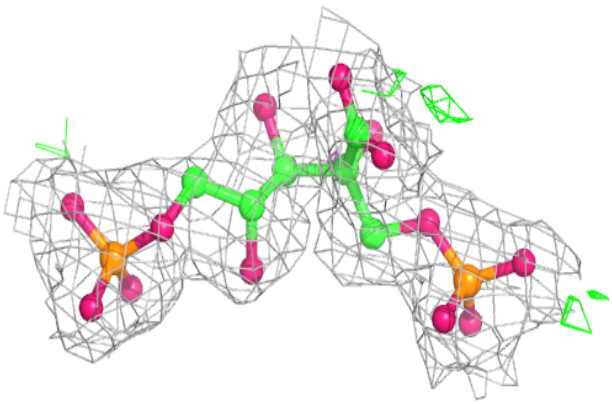


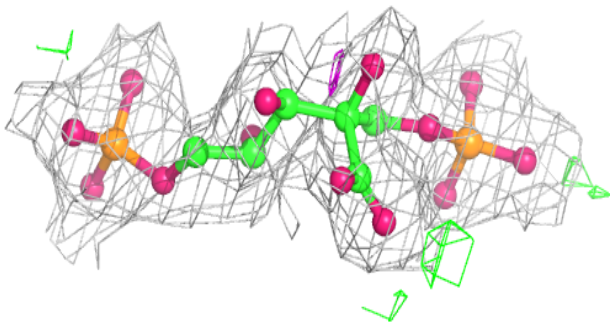


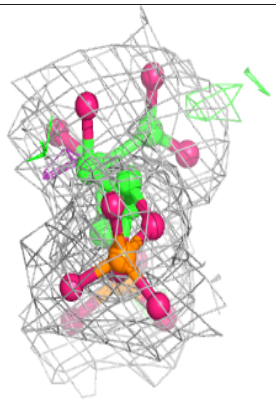


Electron density around CAP B 800:

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

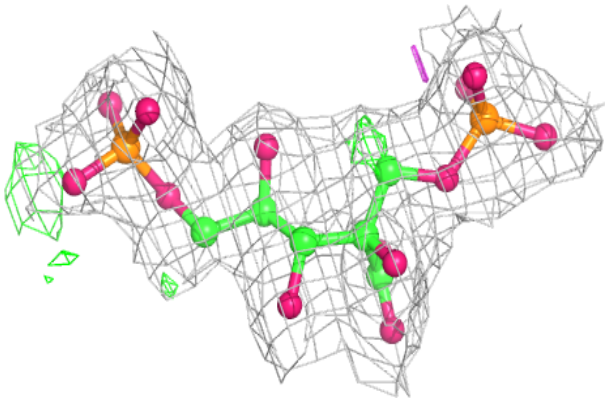


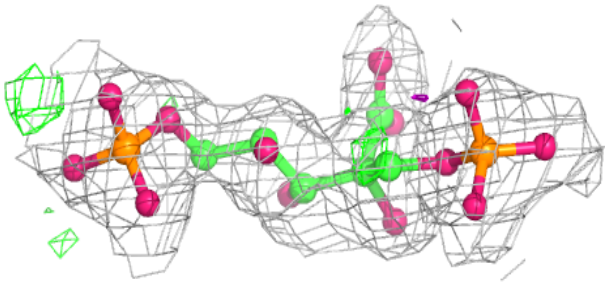


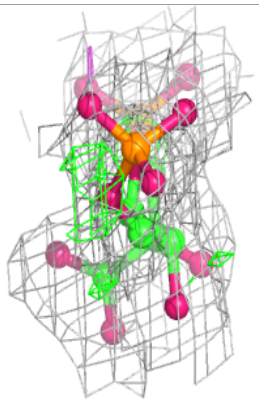


Electron density around CAP E 800:

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

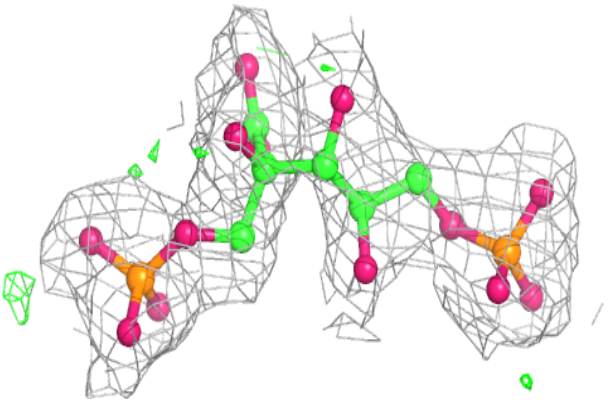


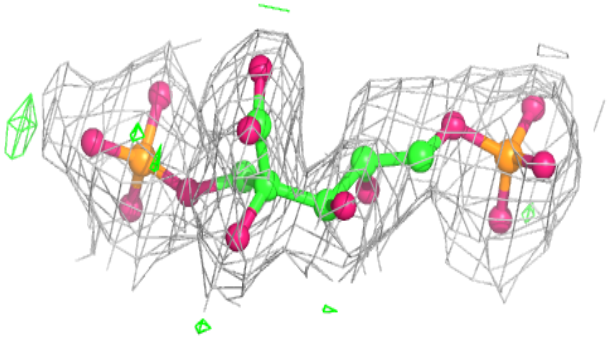


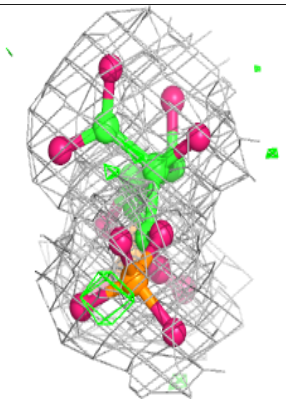


Electron density around CAP C 800:

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

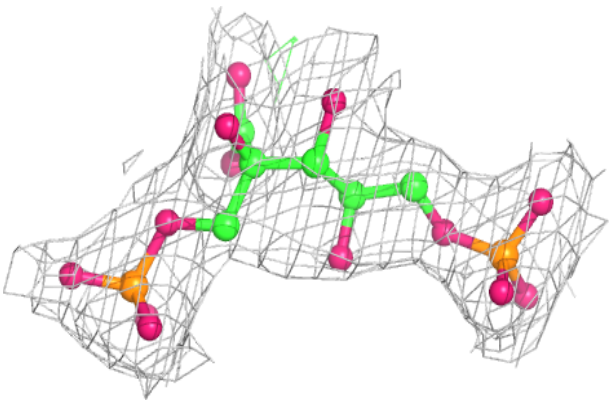


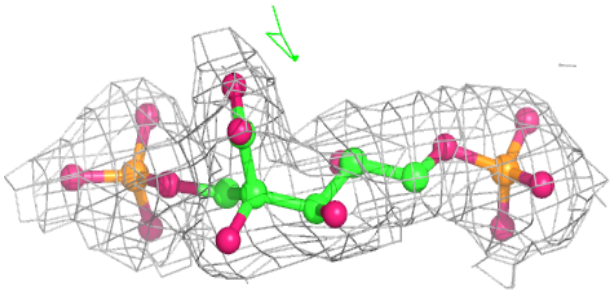


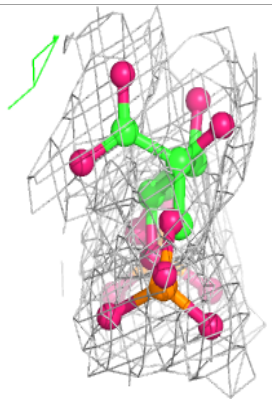


Electron density around CAP A 800:

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

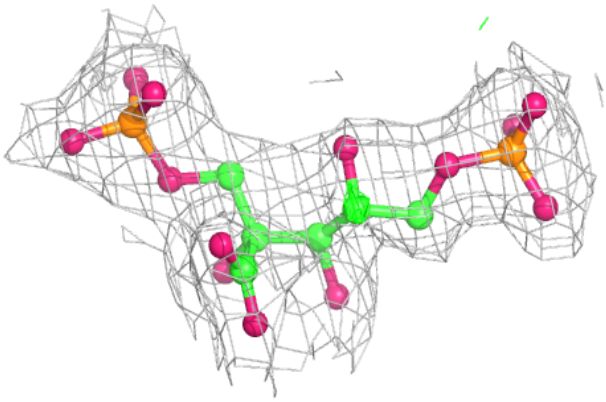


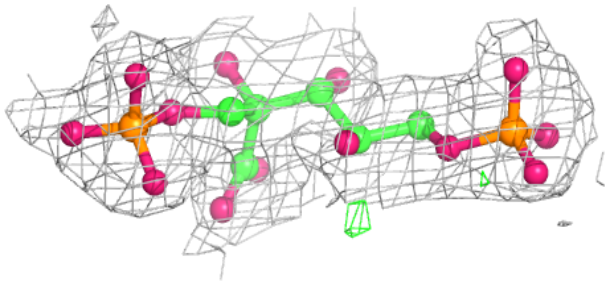




Electron density around CAP D 800:

$2mF_o$-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.