



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 AM UTC

PDB ID : 4LF1 / pdb_00004lf1
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

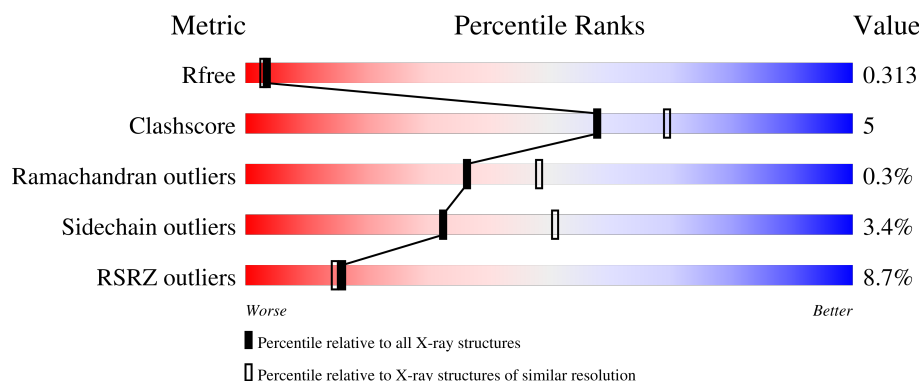
1 Overall quality at a glance

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	9% 85% 8% 5%
1	B	481	8% 86% 7% 6%
1	C	481	9% 81% 11% 6%
1	D	481	8% 83% 10% 5%

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Mol	Chain	Length	Quality of chain
1	E	481	7% 81% 11% 5%
1	F	481	8% 84% 9% 5%

2 Entry composition

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 biphosphate 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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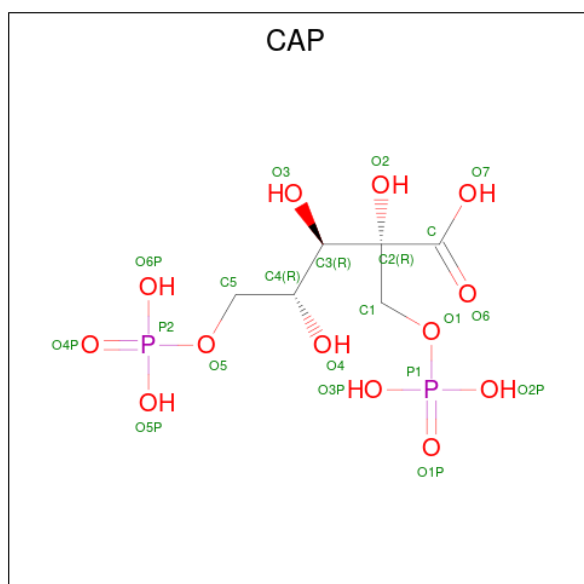
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q6N0W9
D	-19	MET	-	initiating methionine	UNP Q6N0W9
D	-18	GLY	-	expression tag	UNP Q6N0W9
D	-17	SER	-	expression tag	UNP Q6N0W9
D	-16	SER	-	expression tag	UNP Q6N0W9
D	-15	HIS	-	expression tag	UNP Q6N0W9
D	-14	HIS	-	expression 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 (CCD ID: 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	0	0
			21	6	13	2		
2	C	1	Total	C	O	P	0	0
			21	6	13	2		
2	D	1	Total	C	O	P	0	0
			21	6	13	2		
2	E	1	Total	C	O	P	0	0
			21	6	13	2		
2	F	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

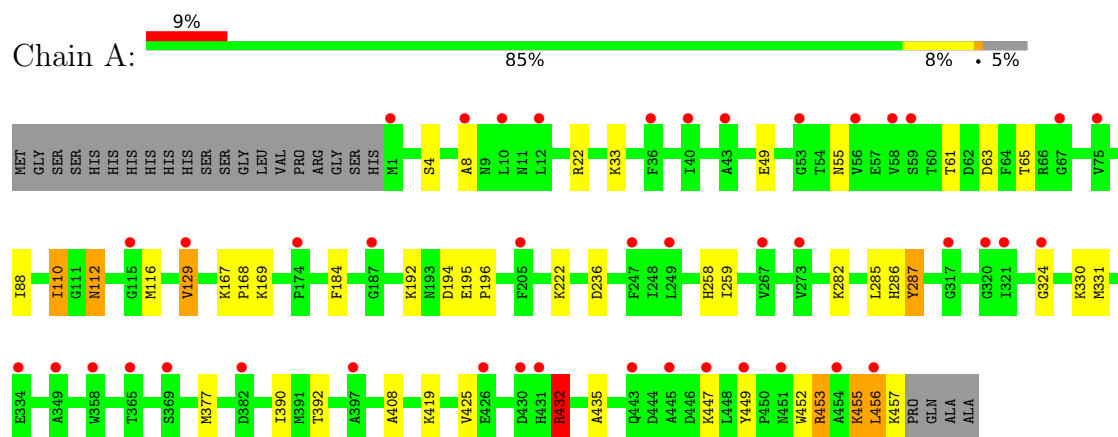
- Molecule 4 is water.

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

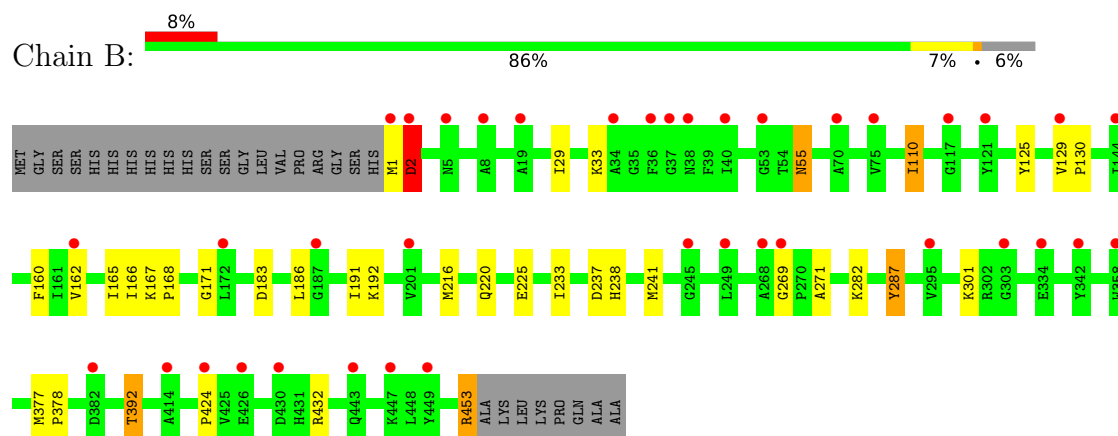
3 Residue-property plots [i](#)

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.

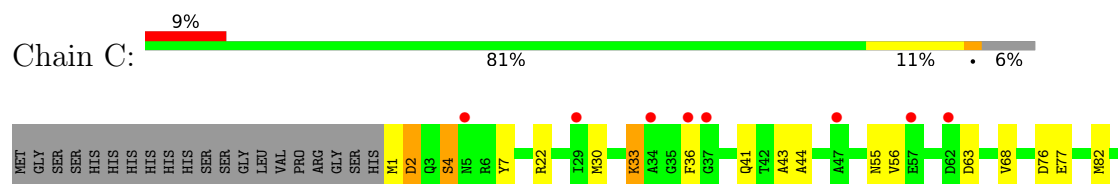
• Molecule 1: Ribulose biphosphate carboxylase

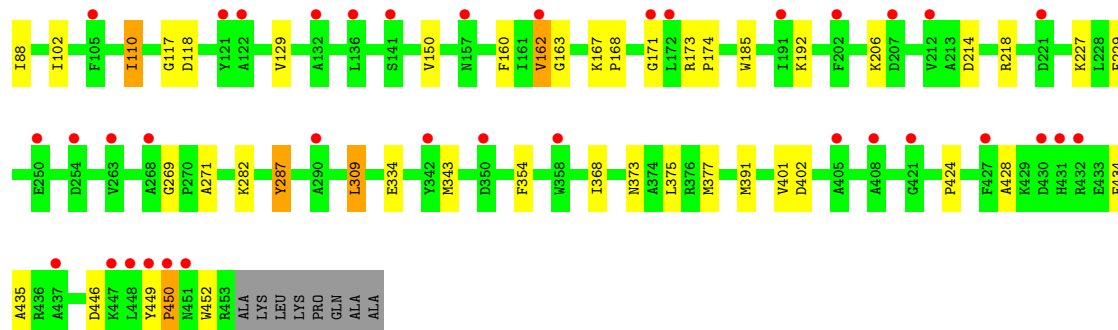


• Molecule 1: Ribulose biphosphate carboxylase

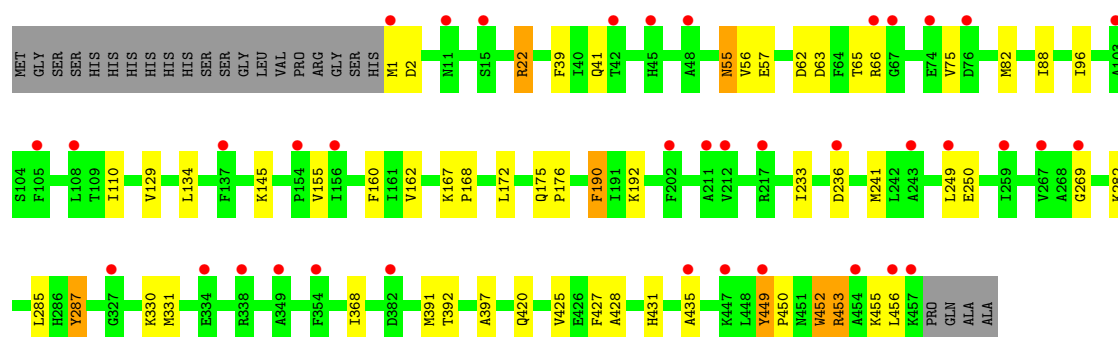
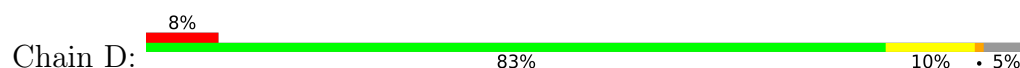


• Molecule 1: Ribulose biphosphate carboxylase

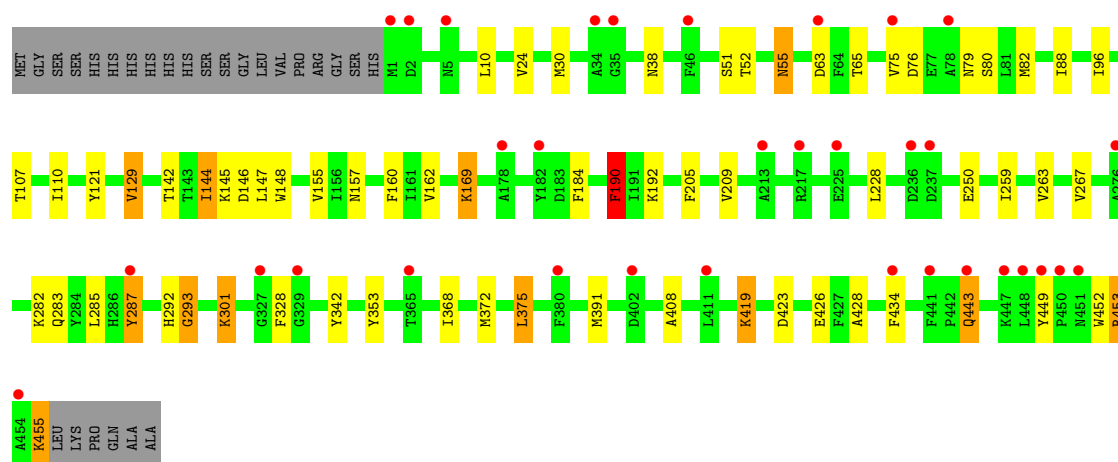
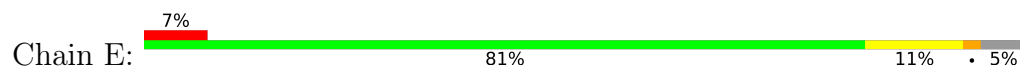




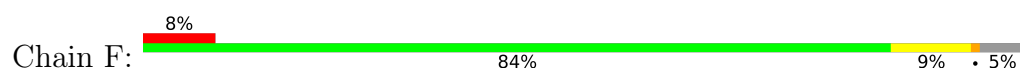
• Molecule 1: Ribulose biphosphate carboxylase

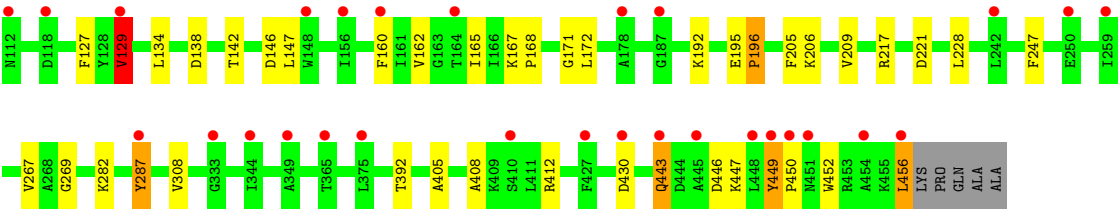


• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase





4 Data and refinement statistics

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 71.29 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.6 (71.29-2.38) 97.6 (71.29-2.38)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (3.93%)	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 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	2/3612 (0.1%)	1.02	7/4886 (0.1%)
1	B	0.87	1/3581 (0.0%)	1.01	10/4846 (0.2%)
1	C	0.88	0/3590	1.10	21/4857 (0.4%)
1	D	0.85	0/3612	1.01	10/4886 (0.2%)
1	E	0.92	1/3604 (0.0%)	1.07	12/4876 (0.2%)
1	F	0.86	0/3614	1.01	6/4889 (0.1%)
All	All	0.88	4/21613 (0.0%)	1.04	66/29240 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	VAL	CA-CB	5.46	1.58	1.54
1	E	129	VAL	CA-CB	5.35	1.58	1.54
1	B	238	HIS	N-CA	-5.27	1.39	1.46
1	A	377	MET	C-O	-5.14	1.19	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	ARG	N-CA-C	10.67	122.49	111.07
1	E	443	GLN	OE1-CD-NE2	-10.12	112.48	122.60
1	B	2	ASP	CA-CB-CG	-9.38	103.22	112.60
1	C	43	ALA	N-CA-C	7.96	120.67	111.11
1	C	449	TYR	O-C-N	7.35	127.98	121.37
1	C	77	GLU	O-C-N	-7.25	114.43	122.12
1	C	77	GLU	CA-C-O	7.13	128.11	120.55
1	E	157	ASN	CB-CA-C	-7.08	102.37	111.86
1	D	452	TRP	N-CA-C	6.90	119.64	111.71
1	E	38	ASN	N-CA-C	6.66	118.44	110.19
1	B	225	GLU	N-CA-C	6.59	120.26	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	450	PRO	N-CA-C	6.53	122.60	113.53
1	C	76	ASP	CB-CA-C	-6.39	103.01	111.82
1	E	190	PHE	N-CA-C	6.32	119.79	109.24
1	B	432	ARG	N-CA-C	6.29	118.14	111.28
1	C	162	VAL	CA-C-N	6.28	126.98	121.58
1	C	162	VAL	C-N-CA	6.28	126.98	121.58
1	D	39	PHE	N-CA-C	6.17	117.67	111.07
1	D	397	ALA	N-CA-C	6.15	119.18	111.24
1	E	267	VAL	N-CA-C	6.15	116.93	110.72
1	E	263	VAL	N-CA-C	6.09	116.64	108.11
1	C	68	VAL	N-CA-C	6.08	117.95	112.17
1	A	390	ILE	CB-CA-C	-6.05	102.45	110.98
1	C	33	LYS	N-CA-C	6.04	118.98	110.23
1	C	269	GLY	CA-C-N	6.02	126.19	119.32
1	C	269	GLY	C-N-CA	6.02	126.19	119.32
1	E	443	GLN	CG-CD-NE2	5.95	125.32	116.40
1	C	229	PHE	N-CA-C	5.91	119.03	109.40
1	C	375	LEU	N-CA-C	5.78	117.58	111.28
1	A	449	TYR	CA-C-N	5.73	127.00	119.84
1	A	449	TYR	C-N-CA	5.73	127.00	119.84
1	C	450	PRO	CA-C-N	-5.71	113.96	123.33
1	C	450	PRO	C-N-CA	-5.71	113.96	123.33
1	E	328	PHE	N-CA-C	5.71	120.08	113.18
1	A	452	TRP	N-CA-C	5.70	118.26	111.71
1	C	452	TRP	N-CA-C	5.69	119.21	112.72
1	F	269	GLY	CA-C-N	5.67	125.79	119.32
1	F	269	GLY	C-N-CA	5.67	125.79	119.32
1	E	342	TYR	N-CA-C	5.63	117.42	111.28
1	C	163	GLY	N-CA-C	5.47	119.61	111.18
1	D	449	TYR	CA-C-N	5.42	126.61	119.84
1	D	449	TYR	C-N-CA	5.42	126.61	119.84
1	D	96	ILE	N-CA-C	5.39	116.12	110.62
1	C	354	PHE	N-CA-C	5.37	118.31	109.72
1	F	449	TYR	CA-C-N	5.36	126.54	119.84
1	F	449	TYR	C-N-CA	5.36	126.54	119.84
1	D	269	GLY	CA-C-N	5.35	125.42	119.32
1	D	269	GLY	C-N-CA	5.35	125.42	119.32
1	F	129	VAL	CB-CA-C	5.35	116.46	110.52
1	D	190	PHE	N-CA-C	5.34	118.16	109.24
1	B	269	GLY	CA-C-N	5.29	125.35	119.32
1	B	269	GLY	C-N-CA	5.29	125.35	119.32
1	A	63	ASP	N-CA-C	5.26	117.76	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	ILE	N-CA-C	5.19	115.92	110.62
1	E	301	LYS	CB-CA-C	-5.18	101.80	110.56
1	C	150	VAL	N-CA-C	5.17	115.89	110.62
1	C	2	ASP	N-CA-C	5.17	117.80	110.10
1	B	238	HIS	CA-CB-CG	-5.12	108.68	113.80
1	E	353	TYR	N-CA-C	5.07	120.32	114.04
1	D	453	ARG	N-CA-C	5.07	116.49	110.97
1	A	259	ILE	N-CA-C	5.03	115.55	108.36
1	F	196	PRO	N-CA-C	5.02	121.05	114.27
1	B	130	PRO	CA-C-N	5.02	126.11	119.84
1	B	130	PRO	C-N-CA	5.02	126.11	119.84
1	B	237	ASP	CA-C-N	5.01	127.24	120.38
1	B	237	ASP	C-N-CA	5.01	127.24	120.38

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	33	0
1	B	3505	0	3372	20	0
1	C	3511	0	3385	36	0
1	D	3536	0	3414	31	0
1	E	3525	0	3396	42	0
1	F	3535	0	3414	35	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
4	D	70	0	0	0	0
4	E	79	0	0	1	0
4	F	89	0	0	1	0
All	All	21750	0	20447	188	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 5.

All (188) 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:HH11	1:E:453:ARG:CB	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:HG3	1:A:453:ARG:HH21	1.38	0.89
1:A:330:LYS:HE3	1:A:331:MET:HE2	1.58	0.85
1:D:330:LYS:HE3	1:D:331:MET:HE2	1.60	0.84
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:HD22	1:E:55:ASN:H	1.33	0.77
1:C:2:ASP:CG	1:C:41:GLN:HG2	2.11	0.75
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:HD3	1:A:432:ARG:O	1.91	0.71
1:A:456:LEU:O	1:A:457:LYS:HB2	1.93	0.68
1:B:1:MET:C	1:B:2:ASP:OD1	2.37	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:H	1:B:55:ASN:HD22	1.44	0.64
1:C:309:LEU:HD12	1:C:309:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LEU:HD12	1:C:309:LEU:C	2.23	0.64
1:C:1:MET:HE1	1:C:56:VAL:HG23	1.80	0.63
1:A:195:GLU:HG2	1:A:196:PRO:HD3	1.80	0.63
1:A:432:ARG:HD3	1:A:432:ARG:C	2.24	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:D:190:PHE:C	1:D:190:PHE:CD1	2.79	0.60
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:H	1:F:55:ASN:HD22	1.49	0.59
1:A:453:ARG:HH21	1:A:453:ARG:CG	2.07	0.58
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:HG3	1:A:453:ARG:NH2	2.16	0.56
1:F:206:LYS:HG2	1:F:247:PHE:CE2	2.40	0.56
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:A:432:ARG:C	1:A:432:ARG:CD	2.79	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:E:30:MET:HB2	1:E:82:MET:HE2	1.88	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:E:190:PHE:CD1	1:E:190:PHE:C	2.87	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:55:ASN:HD22	1:B:55:ASN:N	2.03	0.52
1:B:110:ILE:O	1:B:110:ILE:HG23	2.09	0.52
1:C:373:ASN:O	1:C:377:MET:HG3	2.10	0.52
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.22	0.52
1:B:167:LYS:HA	1:B:168:PRO:C	2.35	0.51
1:D:55:ASN:HD22	1:D:55:ASN:N	2.09	0.51
1:C:36:PHE:CD2	1:C:118:ASP:HB3	2.45	0.51
1:D:55:ASN:H	1:D:55:ASN:ND2	2.08	0.51
1:E:144:ILE:HD13	1:E:148:TRP:CZ2	2.46	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:453:ARG:NH2	2.71	0.50
1:A:167:LYS:NZ	1:A:194:ASP:OD2	2.25	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:HH11	1:B:453:ARG:HG2	1.77	0.48
1:C:446:ASP:O	1:C:450:PRO:HA	2.13	0.48
1:A:110:ILE:O	1:A:110:ILE:HG23	2.13	0.48
1:F:54:THR:HG23	1:F:56:VAL:H	1.77	0.48
1:D:368:ILE:HG21	1:D:391:MET:HE2	1.95	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:55:ASN:H	1:B:55:ASN:ND2	2.12	0.47
1:E:169:LYS:HE2	1:E:169:LYS:HB2	1.77	0.47
1:F:172:LEU:HD23	1:F:172:LEU:HA	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:E:287:TYR:CD1	1:E:287:TYR:C	2.92	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:C:1:MET:HE1	1:C:56:VAL:CG2	2.45	0.46
1:A:49:GLU:HG3	1:A:116:MET:HE3	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:287:TYR:C	1:E:287:TYR:HD1	2.23	0.46
1:C:30:MET:HB2	1:C:82:MET:HE2	1.98	0.45
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:D:1:MET:HE1	1:D:57:GLU:HG3	1.98	0.45
1:F:46:PHE:CG	1:F:82:MET:HE1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:287:TYR:C	1:B:287:TYR:CD1	2.95	0.45
1:E:455:LYS:HE2	1:E:455:LYS:HB3	1.42	0.45
1:C:160:PHE:CE2	1:C:162:VAL:HG22	2.51	0.45
1:F:287:TYR:C	1:F:287:TYR:CD1	2.94	0.45
1:C:271:ALA:HA	1:D:236:ASP:O	2.17	0.45
1:C:287:TYR:C	1:C:287:TYR:CD1	2.95	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:D:1:MET:HE1	1:D:57:GLU:CG	2.46	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
1:A:167:LYS:HA	1:A:168:PRO:C	2.43	0.44
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:D:167:LYS:HA	1:D:168:PRO:C	2.43	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:A:287:TYR:CD1	1:A:287:TYR:C	2.97	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:C:377:MET:HG2	1:C:391:MET:HE1	2.01	0.43
1:D:55:ASN:N	1:D:55:ASN:ND2	2.65	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:167:LYS:HA	1:C:168:PRO:C	2.44	0.43
1:D:287:TYR:C	1:D:287:TYR:CD1	2.97	0.43
1:F:287:TYR:C	1:F:287:TYR:HD1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:TRP:CE3	1:D:453:ARG:HA	2.55	0.42
1:F:456:LEU:N	1:F:456:LEU:HD13	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:F:167:LYS:HA	1:F:168:PRO:C	2.45	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:B:287:TYR:C	1:B:287:TYR:HD1	2.28	0.41
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: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:F:134:LEU:O	1:F:134:LEU:HD12	2.21	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:79:ASN:O	1:E:80:SER:CB	2.50	0.41
1:E:368:ILE:HG21	1:E:391:MET:HE2	2.02	0.41
1:E:372:MET:HB3	1:E:372:MET:HE3	1.71	0.41
1:F:443:GLN:O	1:F:447:LYS:HG3	2.20	0.41
1:D:249:LEU:HD23	1:D:249:LEU:HA	1.87	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:C:2:ASP:OD1	1:C:41:GLN:HG2	2.21	0.41
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:E:30:MET:CB	1:E:82:MET:HE2	2.52	0.40
1:F:412:ARG:HD3	4:F:943:HOH:O	2.21	0.40
1:C:287:TYR:C	1:C:287:TYR:HD1	2.28	0.40
1:C:343:MET:HE3	4:C:921:HOH:O	2.20	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:A:330:LYS:CE	1:A:331:MET:HE2	2.40	0.40
1:D:427:PHE:CE1	1:D:431:HIS:CE1	3.09	0.40
1:A:286:HIS:C	1:A:286:HIS:CD2	2.99	0.40
1:B:29:ILE:HG13	1:B:125:TYR:CE1	2.56	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%)	30	40
1	B	450/481 (94%)	430 (96%)	19 (4%)	1 (0%)	43	56
1	C	451/481 (94%)	430 (95%)	20 (4%)	1 (0%)	43	56
1	D	454/481 (94%)	436 (96%)	16 (4%)	2 (0%)	30	40
1	E	453/481 (94%)	437 (96%)	14 (3%)	2 (0%)	30	40
1	F	454/481 (94%)	438 (96%)	15 (3%)	1 (0%)	43	56
All	All	2716/2886 (94%)	2606 (96%)	101 (4%)	9 (0%)	36	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	293	GLY
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%)	338 (96%)	15 (4%)	26	42
1	B	350/372 (94%)	340 (97%)	10 (3%)	37	57
1	C	351/372 (94%)	342 (97%)	9 (3%)	40	60
1	D	353/372 (95%)	341 (97%)	12 (3%)	32	51
1	E	352/372 (95%)	339 (96%)	13 (4%)	30	47
1	F	353/372 (95%)	340 (96%)	13 (4%)	30	47
All	All	2112/2232 (95%)	2040 (97%)	72 (3%)	32	51

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	55	ASN
1	A	61	THR
1	A	129	VAL
1	A	222	LYS
1	A	258	HIS
1	A	285	LEU
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
1	A	456	LEU
1	B	2	ASP
1	B	33	LYS
1	B	55	ASN
1	B	129	VAL
1	B	282	LYS
1	B	287	TYR
1	B	301	LYS
1	B	392	THR
1	B	424	PRO
1	B	453	ARG
1	C	4	SER
1	C	55	ASN
1	C	63	ASP
1	C	129	VAL
1	C	282	LYS

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Mol	Chain	Res	Type
1	C	287	TYR
1	C	309	LEU
1	C	334	GLU
1	C	424	PRO
1	D	22	ARG
1	D	55	ASN
1	D	56	VAL
1	D	75	VAL
1	D	82	MET
1	D	129	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	129	VAL
1	E	144	ILE
1	E	169	LYS
1	E	190	PHE
1	E	282	LYS
1	E	285	LEU
1	E	287	TYR
1	E	375	LEU
1	E	419	LYS
1	E	453	ARG
1	E	455	LYS
1	F	5	ASN
1	F	33	LYS
1	F	55	ASN
1	F	129	VAL
1	F	165	ILE
1	F	217[A]	ARG
1	F	217[B]	ARG
1	F	282	LYS
1	F	287	TYR
1	F	392	THR
1	F	430	ASP
1	F	443	GLN
1	F	456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	55	ASN
1	A	175	GLN
1	A	316	GLN
1	B	55	ASN
1	C	9	ASN
1	C	55	ASN
1	C	157	ASN
1	D	55	ASN
1	D	316	GLN
1	D	388	ASN
1	D	420	GLN
1	E	55	ASN
1	F	55	ASN
1	F	388	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	B	192	1,3	10,11,12	1.19	1 (10%)	6,12,14	1.01	1 (16%)
1	KCX	D	192	1,3	10,11,12	1.21	1 (10%)	6,12,14	1.13	1 (16%)
1	KCX	F	192	1,3	10,11,12	1.23	1 (10%)	6,12,14	1.04	1 (16%)
1	KCX	E	192	1,3	10,11,12	1.22	1 (10%)	6,12,14	1.24	1 (16%)
1	KCX	C	192	1,3	10,11,12	1.19	1 (10%)	6,12,14	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	A	192	1,3	10,11,12	1.14	1 (10%)	6,12,14	1.42	1 (16%)

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	B	192	1,3	-	0/9/10/12	-
1	KCX	D	192	1,3	-	0/9/10/12	-
1	KCX	F	192	1,3	-	0/9/10/12	-
1	KCX	E	192	1,3	-	0/9/10/12	-
1	KCX	C	192	1,3	-	0/9/10/12	-
1	KCX	A	192	1,3	-	0/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	KCX	CE-NZ	2.78	1.52	1.46
1	F	192	KCX	CE-NZ	2.69	1.52	1.46
1	E	192	KCX	CE-NZ	2.61	1.52	1.46
1	C	192	KCX	CE-NZ	2.49	1.51	1.46
1	D	192	KCX	CE-NZ	2.36	1.51	1.46
1	A	192	KCX	CE-NZ	2.03	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	KCX	OQ1-CX-NZ	-3.21	120.05	124.92
1	E	192	KCX	OQ1-CX-NZ	-2.77	120.72	124.92
1	F	192	KCX	OQ1-CX-NZ	-2.33	121.39	124.92
1	B	192	KCX	OQ1-CX-NZ	-2.27	121.47	124.92
1	D	192	KCX	OQ1-CX-NZ	-2.26	121.49	124.92

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 oligosaccharides 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	A	800	3	18,20,20	0.99	0	23,31,31	1.36	3 (13%)
2	CAP	F	800	3	18,20,20	0.93	0	23,31,31	1.57	2 (8%)
2	CAP	D	800	3	18,20,20	0.91	0	23,31,31	1.43	2 (8%)
2	CAP	E	800	3	18,20,20	0.88	0	23,31,31	1.59	4 (17%)
2	CAP	C	800	3	18,20,20	0.85	0	23,31,31	1.52	4 (17%)
2	CAP	B	800	3	18,20,20	0.94	0	23,31,31	1.66	3 (13%)

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	A	800	3	-	7/29/29/29	-
2	CAP	F	800	3	-	8/29/29/29	-
2	CAP	D	800	3	-	7/29/29/29	-
2	CAP	E	800	3	-	7/29/29/29	-
2	CAP	C	800	3	-	13/29/29/29	-
2	CAP	B	800	3	-	7/29/29/29	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	800	CAP	O7-C-C2	5.75	123.69	114.06
2	B	800	CAP	O7-C-C2	5.33	122.99	114.06
2	E	800	CAP	O7-C-C2	5.24	122.83	114.06
2	C	800	CAP	O7-C-C2	4.78	122.07	114.06
2	D	800	CAP	O7-C-C2	4.70	121.93	114.06
2	A	800	CAP	O7-C-C2	3.78	120.39	114.06
2	B	800	CAP	O1-P1-O1P	3.44	115.74	106.44
2	E	800	CAP	O5P-P2-O5	3.15	114.87	106.67
2	B	800	CAP	O6-C-C2	-2.72	117.25	122.32
2	A	800	CAP	O5P-P2-O5	2.65	113.59	106.67
2	D	800	CAP	O2-C2-C	-2.54	104.30	109.07
2	A	800	CAP	O3P-P1-O1	2.49	113.15	106.67
2	C	800	CAP	O5P-P2-O5	2.35	112.79	106.67
2	C	800	CAP	O1-P1-O1P	2.24	112.49	106.44
2	E	800	CAP	O2-C2-C	-2.20	104.93	109.07
2	C	800	CAP	O3P-P1-O1	2.11	112.18	106.67
2	F	800	CAP	O6-C-C2	-2.04	118.53	122.32
2	E	800	CAP	O6-C-C2	-2.03	118.53	122.32

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	CAP	O6-C-C2-O2
2	B	800	CAP	O6-C-C2-C1
2	B	800	CAP	O7-C-C2-C1
2	B	800	CAP	O6-C-C2-O2
2	B	800	CAP	O7-C-C2-O2
2	B	800	CAP	O3-C3-C4-O4
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	D	800	CAP	O6-C-C2-C1
2	D	800	CAP	O7-C-C2-C1
2	D	800	CAP	O6-C-C2-O2
2	D	800	CAP	O7-C-C2-O2
2	D	800	CAP	O4-C4-C5-O5
2	E	800	CAP	O6-C-C2-O2
2	F	800	CAP	O6-C-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	800	CAP	O4-C4-C5-O5
2	A	800	CAP	O7-C-C2-C1
2	F	800	CAP	O7-C-C2-C1
2	D	800	CAP	C3-C4-C5-O5
2	F	800	CAP	C3-C4-C5-O5
2	A	800	CAP	O7-C-C2-O2
2	F	800	CAP	O7-C-C2-O2
2	C	800	CAP	O6-C-C2-O2
2	C	800	CAP	O6-C-C2-C3
2	E	800	CAP	O6-C-C2-C3
2	F	800	CAP	O6-C-C2-C1
2	A	800	CAP	O2-C2-C3-C4
2	B	800	CAP	O2-C2-C3-C4
2	C	800	CAP	O2-C2-C3-C4
2	D	800	CAP	O2-C2-C3-C4
2	E	800	CAP	O2-C2-C3-C4
2	F	800	CAP	O2-C2-C3-C4
2	C	800	CAP	O1-C1-C2-C3
2	A	800	CAP	O6-C-C2-C1
2	C	800	CAP	O7-C-C2-C3
2	E	800	CAP	O7-C-C2-C3
2	E	800	CAP	O3-C3-C4-O4
2	E	800	CAP	O7-C-C2-O2
2	A	800	CAP	O6-C-C2-C3
2	E	800	CAP	C4-C5-O5-P2
2	A	800	CAP	O4-C4-C5-O5
2	F	800	CAP	O1-C1-C2-O2
2	C	800	CAP	O7-C-C2-O2
2	B	800	CAP	C2-C3-C4-O4

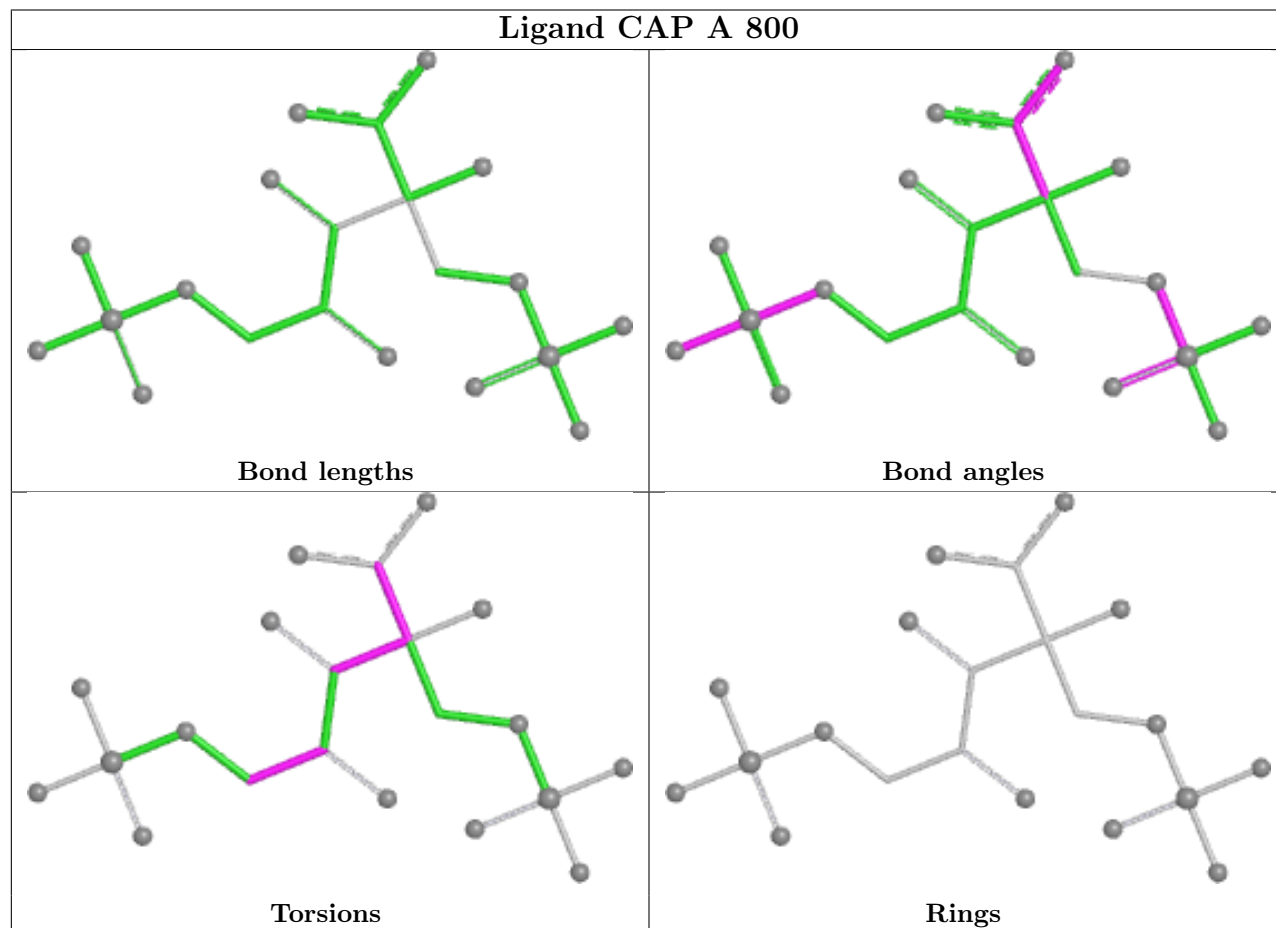
There are no ring outliers.

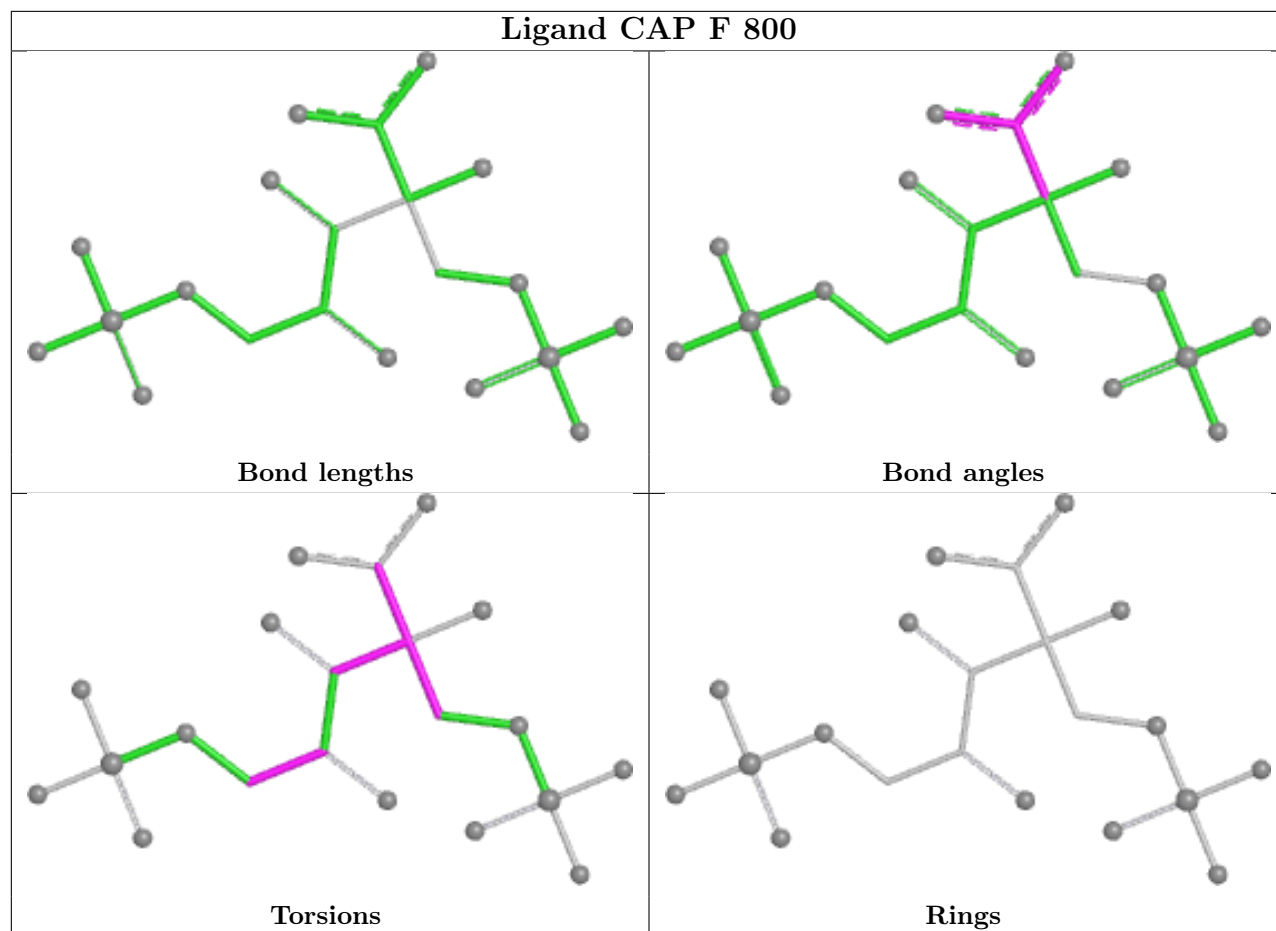
3 monomers are involved in 3 short contacts:

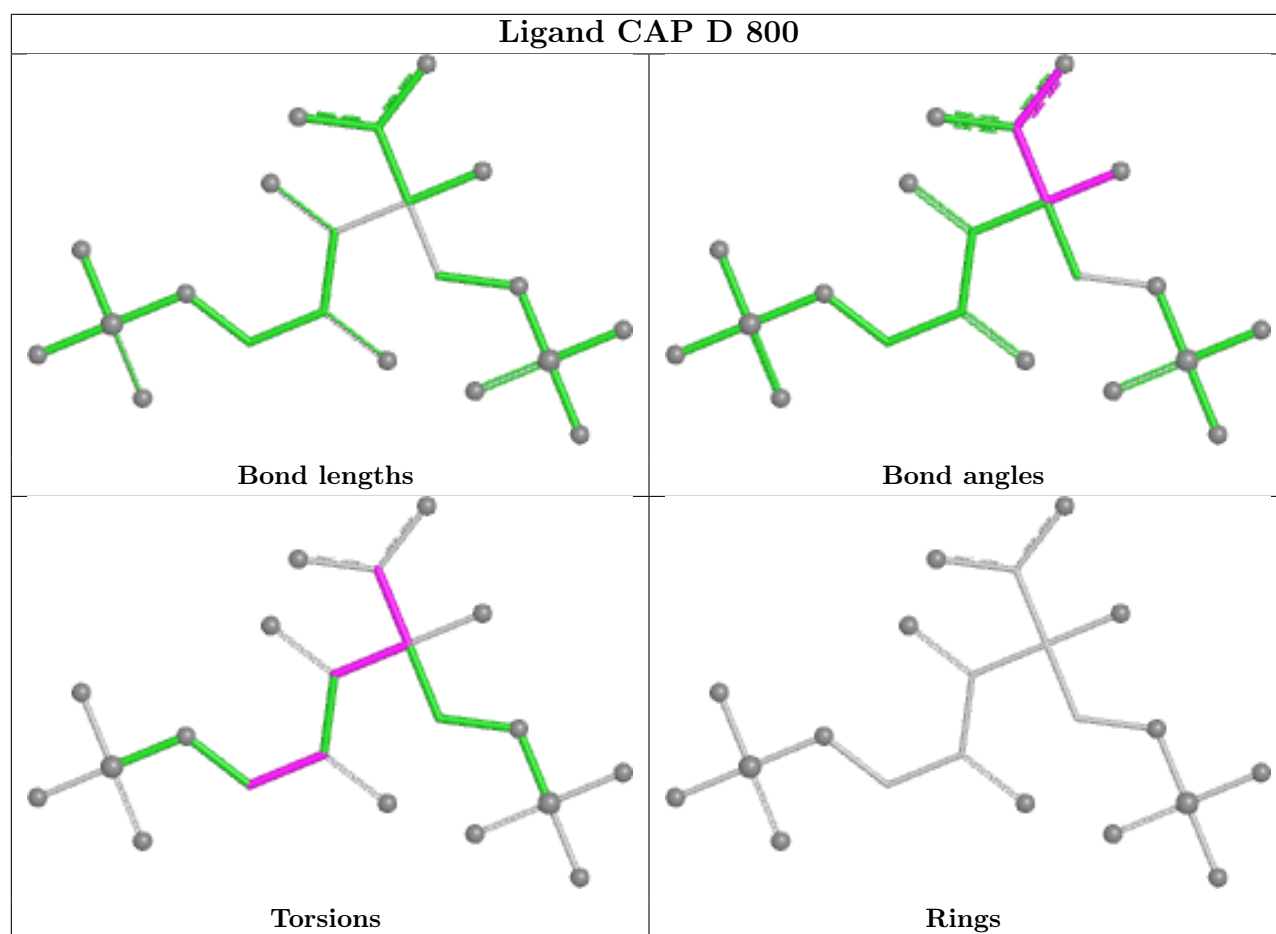
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	800	CAP	1	0
2	C	800	CAP	1	0
2	B	800	CAP	1	0

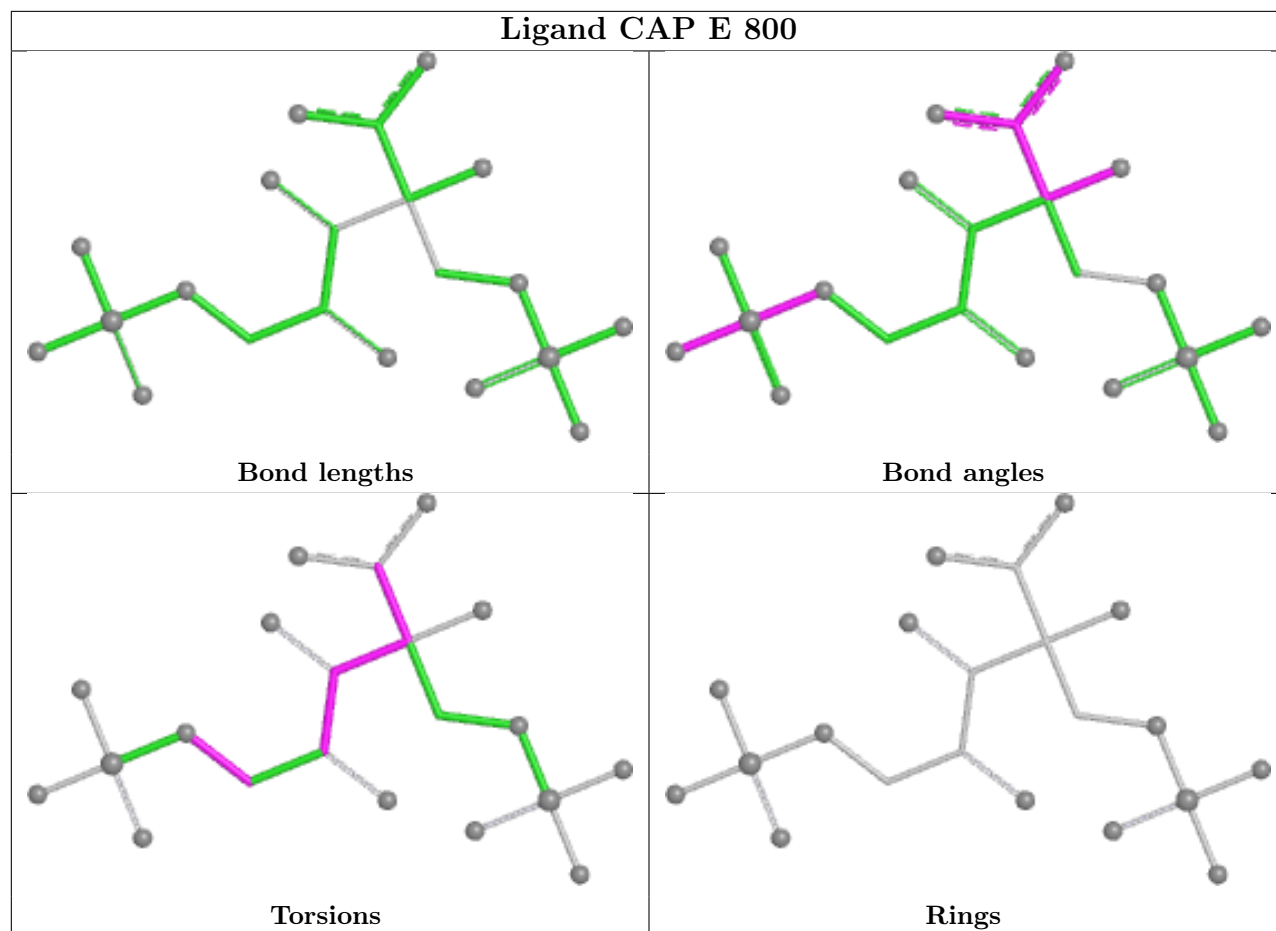
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

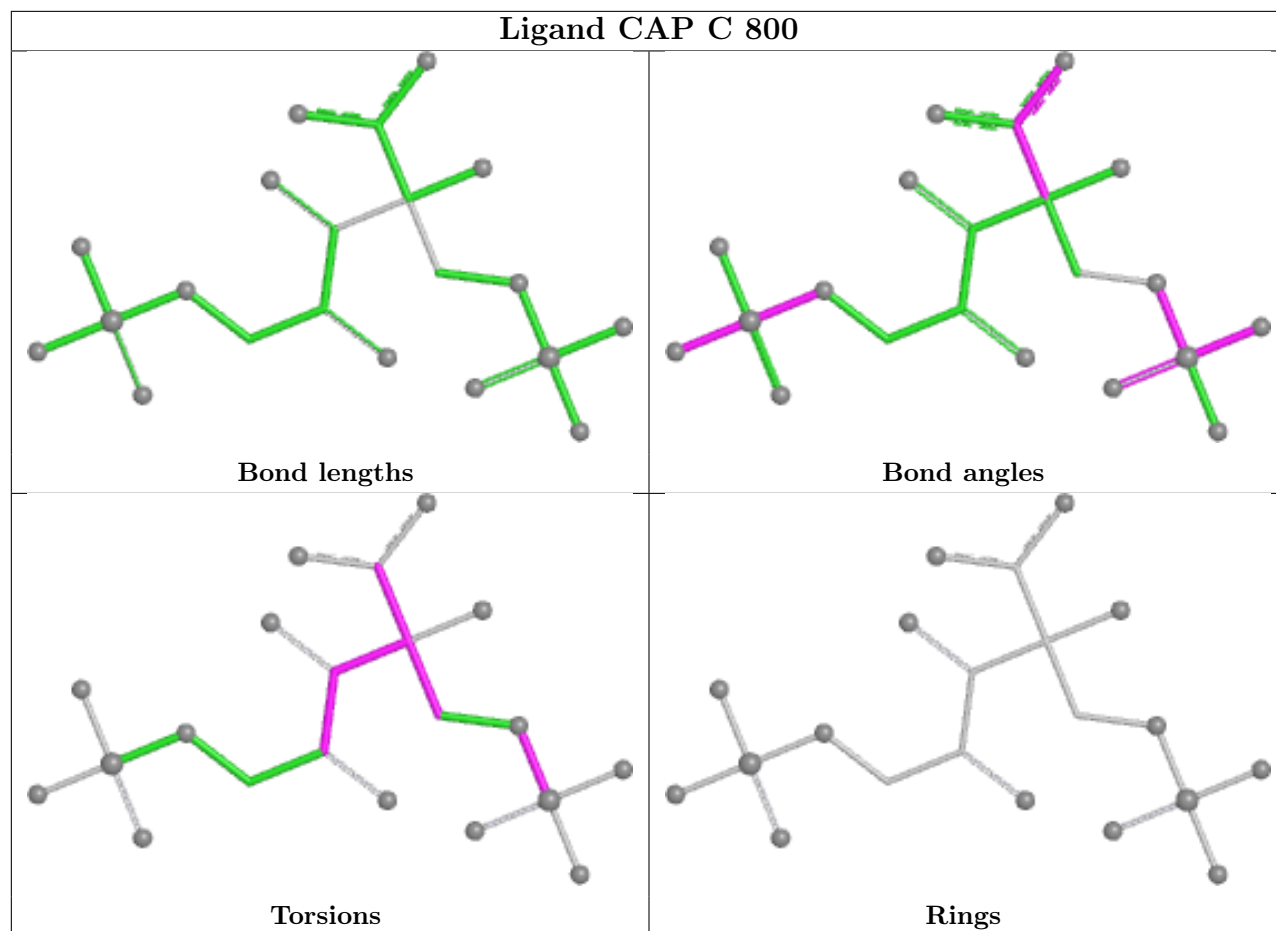
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

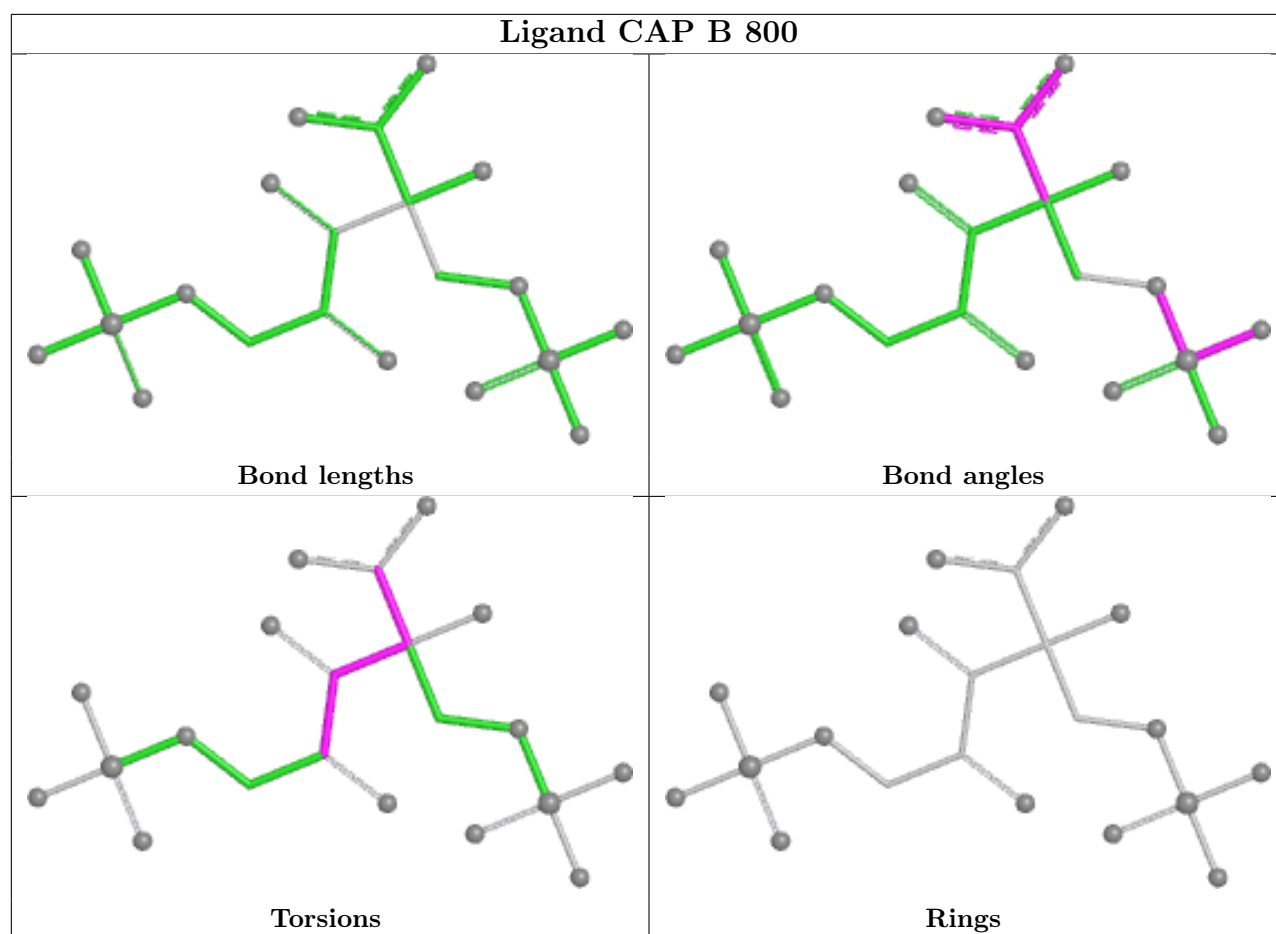












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	456/481 (94%)	1.11	43 (9%) 14 13	5, 13, 26, 54	0
1	B	452/481 (93%)	1.08	38 (8%) 17 15	5, 13, 26, 49	0
1	C	452/481 (93%)	1.06	44 (9%) 13 12	6, 13, 28, 49	2 (0%)
1	D	456/481 (94%)	1.08	38 (8%) 17 16	4, 13, 26, 74	3 (0%)
1	E	454/481 (94%)	1.04	33 (7%) 21 20	6, 13, 27, 47	1 (0%)
1	F	455/481 (94%)	1.06	40 (8%) 15 14	7, 13, 27, 54	2 (0%)
All	All	2725/2886 (94%)	1.07	236 (8%) 16 15	4, 13, 27, 74	8 (0%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	ALA	5.4
1	D	454	ALA	5.4
1	D	1	MET	4.9
1	B	414	ALA	4.7
1	F	37	GLY	4.5
1	B	268	ALA	4.3
1	E	451	ASN	4.1
1	E	217	ARG	4.0
1	C	450	PRO	3.9
1	D	217	ARG	3.8
1	C	37	GLY	3.8
1	E	449	TYR	3.7
1	C	34	ALA	3.7
1	C	171	GLY	3.6
1	D	243	ALA	3.6
1	C	448	LEU	3.5
1	C	342	TYR	3.5
1	D	334	GLU	3.4
1	F	448	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	3.4
1	C	421	GLY	3.4
1	C	432	ARG	3.3
1	E	78	ALA	3.3
1	E	454	ALA	3.3
1	A	1	MET	3.3
1	B	449	TYR	3.3
1	B	34	ALA	3.2
1	D	338	ARG	3.2
1	D	349	ALA	3.2
1	F	349	ALA	3.2
1	D	456	LEU	3.2
1	F	450	PRO	3.2
1	B	430	ASP	3.2
1	C	62	ASP	3.2
1	F	187	GLY	3.1
1	E	365	THR	3.1
1	C	36	PHE	3.1
1	E	178	ALA	3.1
1	C	430	ASP	3.1
1	A	445	ALA	3.0
1	C	172	LEU	3.0
1	E	450	PRO	3.0
1	F	454	ALA	2.9
1	A	443	GLN	2.9
1	A	449	TYR	2.9
1	F	449	TYR	2.9
1	A	334	GLU	2.9
1	D	66	ARG	2.9
1	E	448	LEU	2.9
1	C	350	ASP	2.9
1	B	37	GLY	2.8
1	A	10	LEU	2.8
1	C	105	PHE	2.8
1	F	57	GLU	2.8
1	E	443	GLN	2.8
1	B	36	PHE	2.8
1	B	53	GLY	2.8
1	F	375	LEU	2.8
1	D	382	ASP	2.8
1	C	427	PHE	2.8
1	E	236	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	447	LYS	2.7
1	C	447	LYS	2.7
1	C	136	LEU	2.7
1	C	451	ASN	2.7
1	F	430	ASP	2.7
1	F	333	GLY	2.7
1	D	15	SER	2.7
1	B	443	GLN	2.7
1	F	112	ASN	2.7
1	A	317	GLY	2.7
1	B	303	GLY	2.7
1	E	1	MET	2.7
1	A	12	LEU	2.7
1	A	447	LYS	2.6
1	A	451	ASN	2.6
1	C	47	ALA	2.6
1	C	207	ASP	2.6
1	F	427	PHE	2.6
1	A	75	VAL	2.6
1	D	212	VAL	2.6
1	A	365	THR	2.6
1	A	8	ALA	2.6
1	D	327	GLY	2.6
1	E	75	VAL	2.6
1	C	449	TYR	2.6
1	E	182	TYR	2.6
1	A	320	GLY	2.5
1	D	156	ILE	2.5
1	C	121	TYR	2.5
1	D	48	ALA	2.5
1	E	34	ALA	2.5
1	A	369	SER	2.5
1	F	410	SER	2.5
1	B	1	MET	2.5
1	B	2	ASP	2.5
1	C	405	ALA	2.5
1	D	211	ALA	2.5
1	E	447	LYS	2.5
1	F	178	ALA	2.5
1	B	117	GLY	2.5
1	F	156	ILE	2.4
1	A	67	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	GLU	2.4
1	C	268	ALA	2.4
1	C	290	ALA	2.4
1	D	67	GLY	2.4
1	D	103	ALA	2.4
1	B	40	ILE	2.4
1	D	202	PHE	2.4
1	D	249	LEU	2.4
1	A	431	HIS	2.4
1	B	424	PRO	2.4
1	F	164	THR	2.4
1	A	129	VAL	2.4
1	F	64	PHE	2.4
1	F	72	VAL	2.4
1	D	108	LEU	2.4
1	B	342	TYR	2.3
1	A	174	PRO	2.3
1	E	327	GLY	2.3
1	E	329	GLY	2.3
1	D	435	ALA	2.3
1	D	457	LYS	2.3
1	B	172	LEU	2.3
1	D	76	ASP	2.3
1	B	269	GLY	2.3
1	F	365	THR	2.3
1	F	40	ILE	2.3
1	B	201	VAL	2.3
1	B	426	GLU	2.3
1	C	212	VAL	2.3
1	D	105	PHE	2.3
1	B	38	ASN	2.3
1	C	221	ASP	2.3
1	D	447	LYS	2.3
1	E	402	ASP	2.3
1	A	53	GLY	2.3
1	E	35	GLY	2.3
1	E	287	TYR	2.3
1	A	349	ALA	2.3
1	C	141	SER	2.3
1	C	191	ILE	2.3
1	A	267	VAL	2.3
1	A	273	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	162	VAL	2.3
1	C	162	VAL	2.3
1	D	354	PHE	2.3
1	E	441	PHE	2.3
1	F	456	LEU	2.3
1	C	157	ASN	2.3
1	B	245	GLY	2.3
1	D	449	TYR	2.3
1	F	287	TYR	2.3
1	B	8	ALA	2.3
1	F	445	ALA	2.3
1	F	250	GLU	2.3
1	F	160	PHE	2.2
1	A	382	ASP	2.2
1	A	358	TRP	2.2
1	B	358	TRP	2.2
1	A	430	ASP	2.2
1	B	5	ASN	2.2
1	F	118	ASP	2.2
1	B	121	TYR	2.2
1	F	259	ILE	2.2
1	F	242	LEU	2.2
1	B	129	VAL	2.2
1	B	19	ALA	2.2
1	C	408	ALA	2.2
1	F	43	ALA	2.2
1	A	249	LEU	2.2
1	C	29	ILE	2.2
1	B	295	VAL	2.2
1	C	5	ASN	2.2
1	C	263	VAL	2.2
1	B	187	GLY	2.2
1	A	397	ALA	2.2
1	C	132	ALA	2.2
1	F	60	THR	2.2
1	A	40	ILE	2.1
1	C	358	TRP	2.1
1	E	411	LEU	2.1
1	F	344	ILE	2.1
1	F	148	TRP	2.1
1	A	58	VAL	2.1
1	D	11	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	PHE	2.1
1	A	205	PHE	2.1
1	A	426	GLU	2.1
1	D	137	PHE	2.1
1	E	434	PHE	2.1
1	F	443	GLN	2.1
1	C	122	ALA	2.1
1	C	57	GLU	2.1
1	C	254	ASP	2.1
1	D	74	GLU	2.1
1	E	2	ASP	2.1
1	E	225	GLU	2.1
1	B	75	VAL	2.1
1	D	154	PRO	2.1
1	D	267	VAL	2.1
1	F	129	VAL	2.1
1	E	380	PHE	2.1
1	F	59	SER	2.1
1	A	321	ILE	2.1
1	E	237	ASP	2.1
1	A	247	PHE	2.1
1	E	276	ALA	2.1
1	F	78	ALA	2.1
1	D	45	HIS	2.1
1	B	144	ILE	2.1
1	D	236	ASP	2.1
1	E	63	ASP	2.1
1	A	187	GLY	2.1
1	C	202	PHE	2.1
1	F	67	GLY	2.1
1	A	59	SER	2.0
1	A	43	ALA	2.0
1	B	249	LEU	2.0
1	E	5	ASN	2.0
1	F	451	ASN	2.0
1	A	56	VAL	2.0
1	A	115	GLY	2.0
1	A	324	GLY	2.0
1	D	269	GLY	2.0
1	E	46	PHE	2.0
1	C	250	GLU	2.0
1	D	42	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	70	ALA	2.0
1	C	437	ALA	2.0
1	E	213	ALA	2.0
1	C	431	HIS	2.0
1	A	456	LEU	2.0
1	B	382	ASP	2.0
1	D	259	ILE	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, 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
1	KCX	D	192	12/13	0.79	0.13	9,11,22,25	0
1	KCX	A	192	12/13	0.80	0.14	9,11,22,25	0
1	KCX	C	192	12/13	0.85	0.12	9,10,22,25	0
1	KCX	F	192	12/13	0.86	0.10	9,11,22,25	0
1	KCX	E	192	12/13	0.89	0.09	9,11,22,25	0
1	KCX	B	192	12/13	0.89	0.09	9,11,22,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

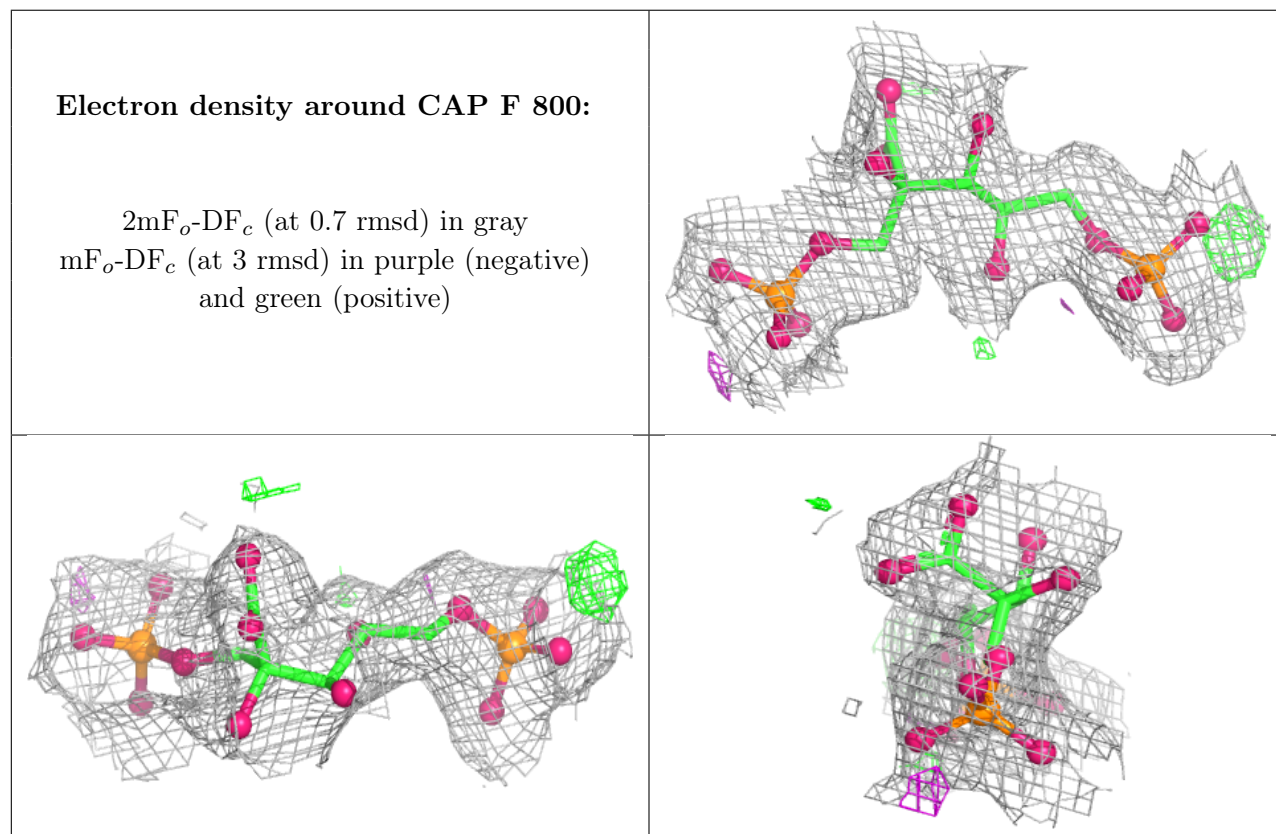
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	C	801	1/1	0.89	0.07	33,33,33,33	0
2	CAP	F	800	21/21	0.90	0.10	4,16,26,29	0
3	MG	B	801	1/1	0.91	0.05	33,33,33,33	0
2	CAP	E	800	21/21	0.92	0.09	2,13,19,26	0
2	CAP	C	800	21/21	0.92	0.09	2,12,18,24	0

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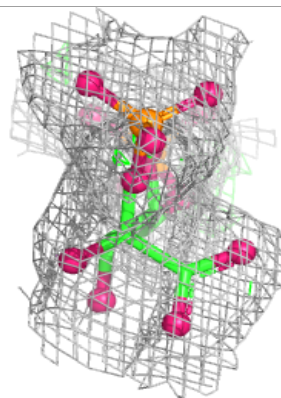
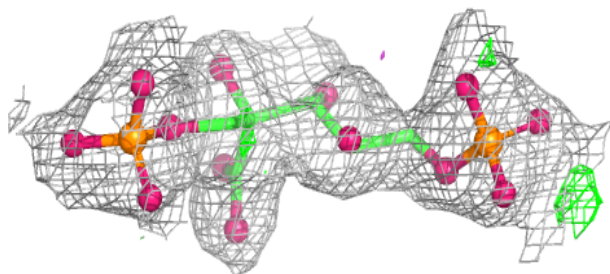
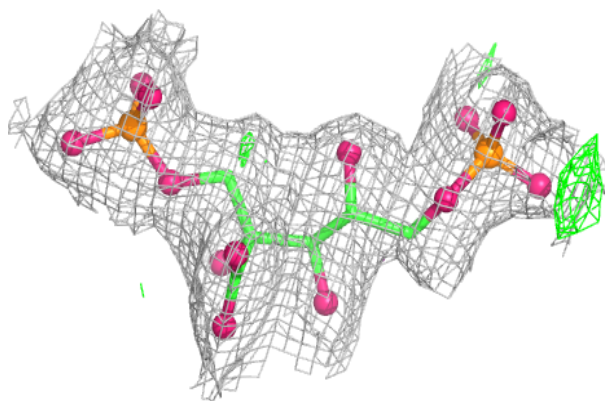
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	F	801	1/1	0.93	0.08	11,11,11,11	0
3	MG	D	801	1/1	0.94	0.04	13,13,13,13	0
2	CAP	B	800	21/21	0.94	0.09	2,10,16,22	0
2	CAP	A	800	21/21	0.95	0.08	2,12,20,26	0
2	CAP	D	800	21/21	0.95	0.08	4,15,24,34	0
3	MG	E	801	1/1	0.96	0.03	21,21,21,21	0
3	MG	A	801	1/1	0.97	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.

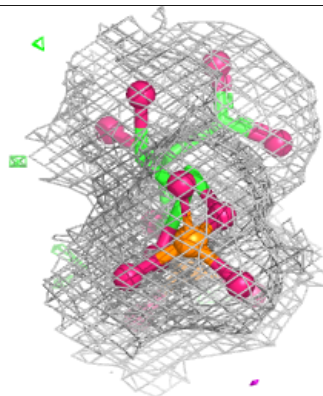
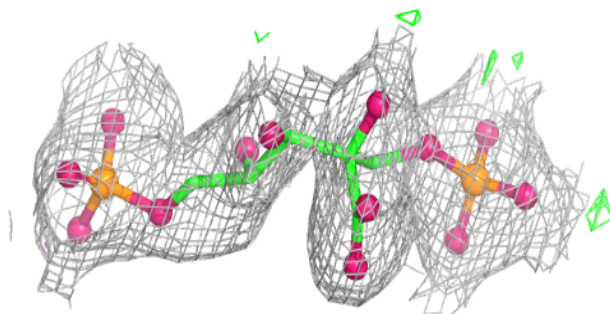
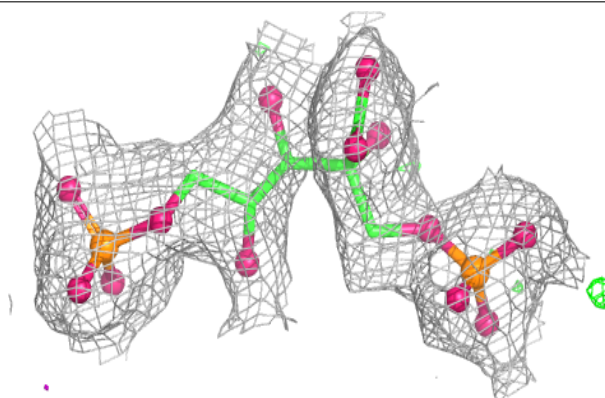


Electron density around CAP E 800:

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

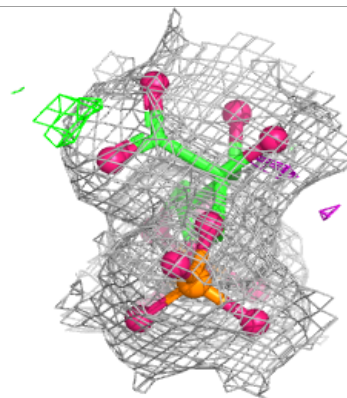
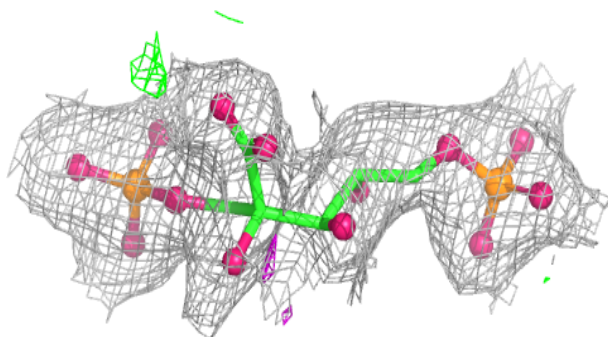
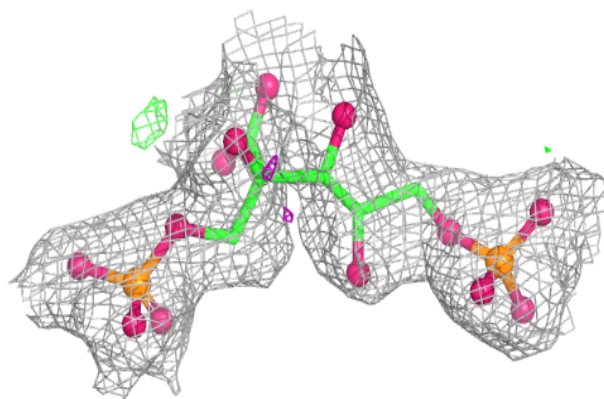
**Electron density around CAP C 800:**

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

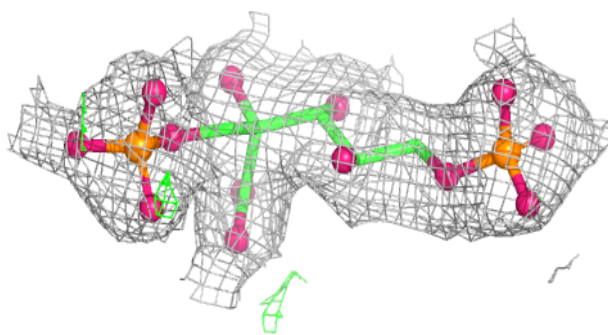
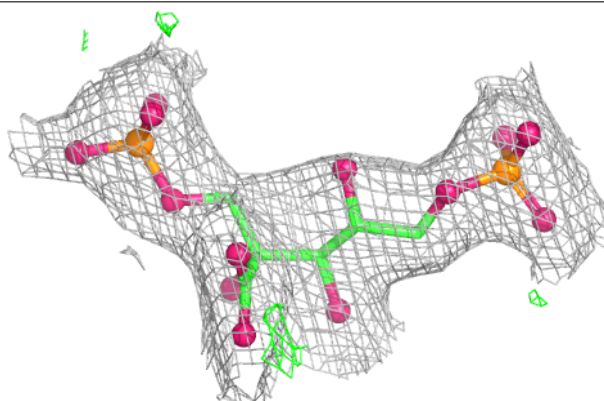


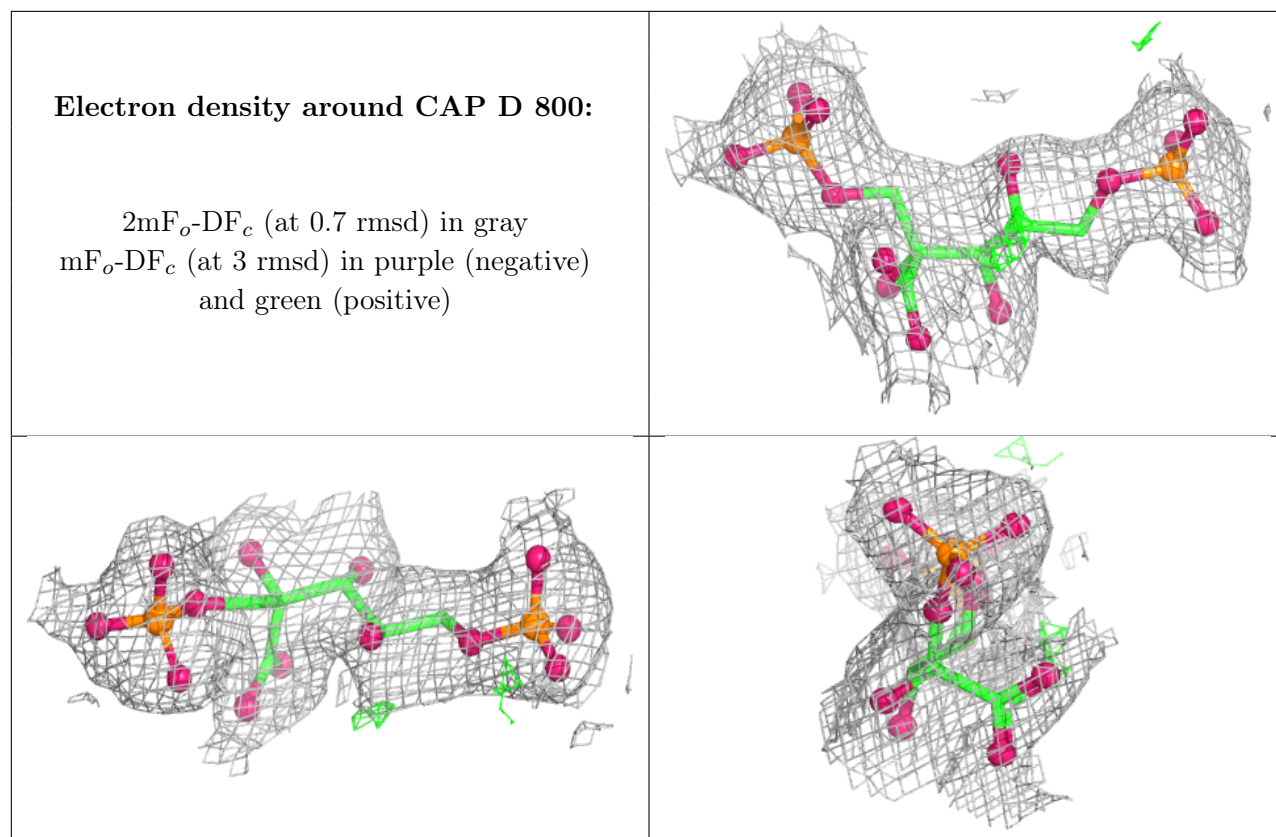
Electron density around CAP B 800:

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

**Electron density around CAP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.