



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:14 PM UTC

PDB ID : 3KDN / pdb_00003kdn
Title : Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-10-23
Resolution : 2.09 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

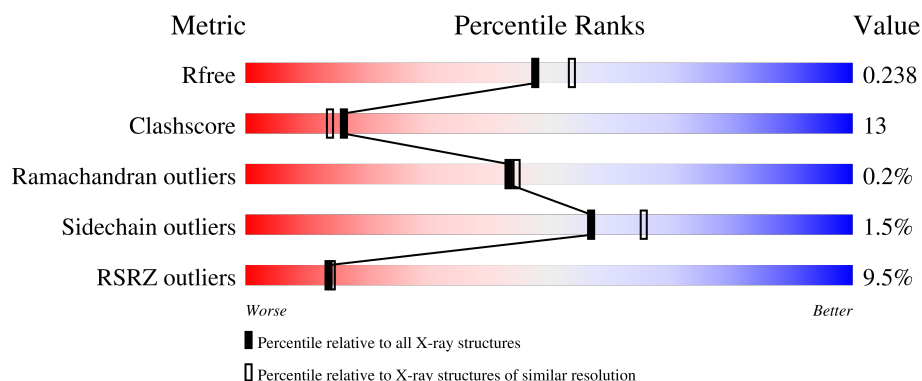
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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.



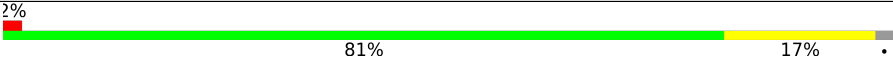
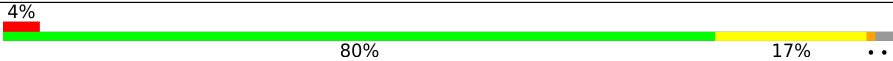
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	444	42% 56% 41% ..
1	B	444	% 79% 19% .
1	C	444	3% 78% 20% .
1	D	444	2% 79% 19% .
1	E	444	7% 78% 20% .

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Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36999 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	437	Total	C	N	O	S	0	0	0
			3349	2145	577	617	10			
1	B	437	Total	C	N	O	S	0	0	0
			3430	2201	588	631	10			
1	C	437	Total	C	N	O	S	0	0	0
			3417	2195	585	627	10			
1	D	437	Total	C	N	O	S	0	0	0
			3421	2196	586	629	10			
1	E	438	Total	C	N	O	S	0	0	0
			3428	2197	586	635	10			
1	F	437	Total	C	N	O	S	0	0	0
			3404	2185	586	623	10			
1	G	437	Total	C	N	O	S	0	0	0
			3433	2204	588	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3396	2182	584	620	10			
1	I	436	Total	C	N	O	S	0	0	0
			3421	2195	586	630	10			
1	J	437	Total	C	N	O	S	0	0	0
			3428	2199	586	633	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	engineered mutation	UNP O93627
A	327	ARG	LYS	engineered mutation	UNP O93627
A	328	ASP	TRP	engineered mutation	UNP O93627
A	329	ILE	ASP	engineered mutation	UNP O93627
A	330	THR	VAL	engineered mutation	UNP O93627
B	326	GLU	GLY	engineered mutation	UNP O93627
B	327	ARG	LYS	engineered mutation	UNP O93627
B	328	ASP	TRP	engineered mutation	UNP O93627
B	329	ILE	ASP	engineered mutation	UNP O93627

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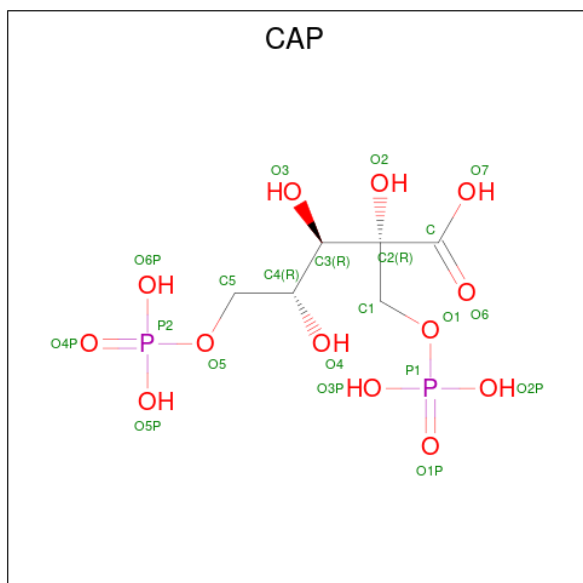
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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	engineered mutation	UNP O93627
C	326	GLU	GLY	engineered mutation	UNP O93627
C	327	ARG	LYS	engineered mutation	UNP O93627
C	328	ASP	TRP	engineered mutation	UNP O93627
C	329	ILE	ASP	engineered mutation	UNP O93627
C	330	THR	VAL	engineered mutation	UNP O93627
D	326	GLU	GLY	engineered mutation	UNP O93627
D	327	ARG	LYS	engineered mutation	UNP O93627
D	328	ASP	TRP	engineered mutation	UNP O93627
D	329	ILE	ASP	engineered mutation	UNP O93627
D	330	THR	VAL	engineered mutation	UNP O93627
E	326	GLU	GLY	engineered mutation	UNP O93627
E	327	ARG	LYS	engineered mutation	UNP O93627
E	328	ASP	TRP	engineered mutation	UNP O93627
E	329	ILE	ASP	engineered mutation	UNP O93627
E	330	THR	VAL	engineered mutation	UNP O93627
F	326	GLU	GLY	engineered mutation	UNP O93627
F	327	ARG	LYS	engineered mutation	UNP O93627
F	328	ASP	TRP	engineered mutation	UNP O93627
F	329	ILE	ASP	engineered mutation	UNP O93627
F	330	THR	VAL	engineered mutation	UNP O93627
G	326	GLU	GLY	engineered mutation	UNP O93627
G	327	ARG	LYS	engineered mutation	UNP O93627
G	328	ASP	TRP	engineered mutation	UNP O93627
G	329	ILE	ASP	engineered mutation	UNP O93627
G	330	THR	VAL	engineered mutation	UNP O93627
H	326	GLU	GLY	engineered mutation	UNP O93627
H	327	ARG	LYS	engineered mutation	UNP O93627
H	328	ASP	TRP	engineered mutation	UNP O93627
H	329	ILE	ASP	engineered mutation	UNP O93627
H	330	THR	VAL	engineered mutation	UNP O93627
I	326	GLU	GLY	engineered mutation	UNP O93627
I	327	ARG	LYS	engineered mutation	UNP O93627
I	328	ASP	TRP	engineered mutation	UNP O93627
I	329	ILE	ASP	engineered mutation	UNP O93627
I	330	THR	VAL	engineered mutation	UNP O93627
J	326	GLU	GLY	engineered mutation	UNP O93627
J	327	ARG	LYS	engineered mutation	UNP O93627
J	328	ASP	TRP	engineered mutation	UNP O93627
J	329	ILE	ASP	engineered mutation	UNP O93627
J	330	THR	VAL	engineered mutation	UNP O93627

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0

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



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

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

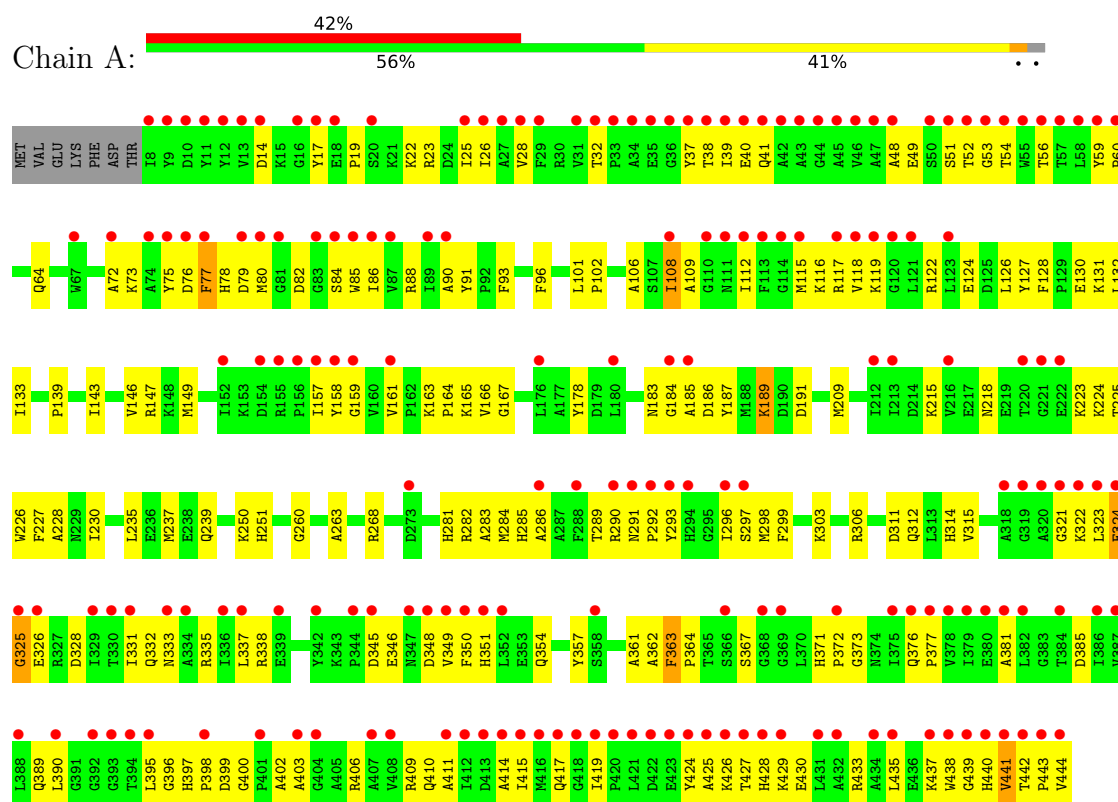
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	290	Total	O	0	0
			290	290		
4	C	311	Total	O	0	0
			311	311		
4	D	308	Total	O	0	0
			308	308		
4	E	258	Total	O	0	0
			258	258		
4	F	268	Total	O	0	0
			268	268		
4	G	267	Total	O	0	0
			267	267		
4	H	185	Total	O	0	0
			185	185		
4	I	291	Total	O	0	0
			291	291		
4	J	301	Total	O	0	0
			301	301		

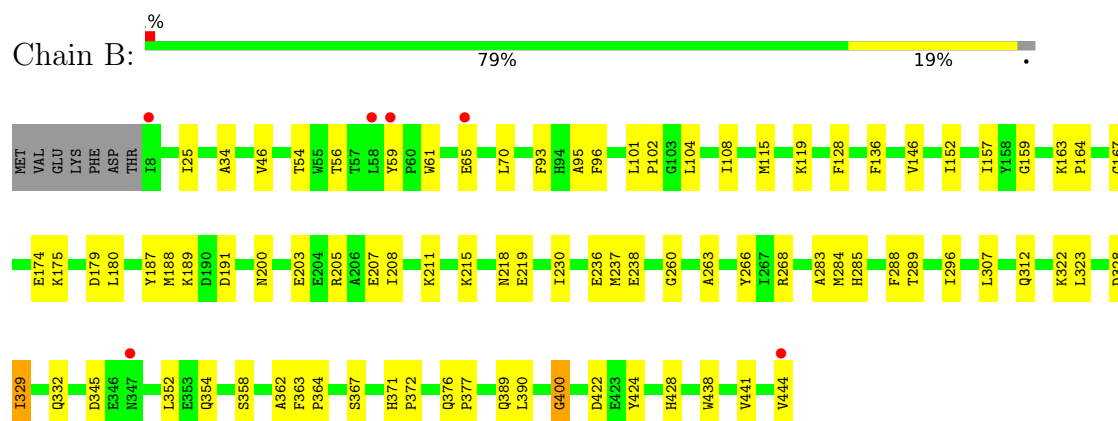
3 Residue-property plots

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



[illegible]

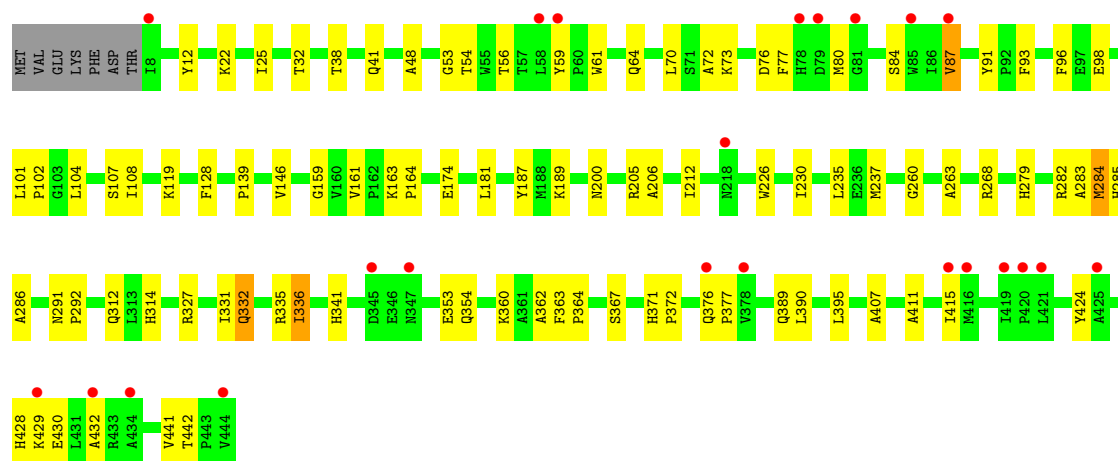
Chain D:

2% 79% 19%

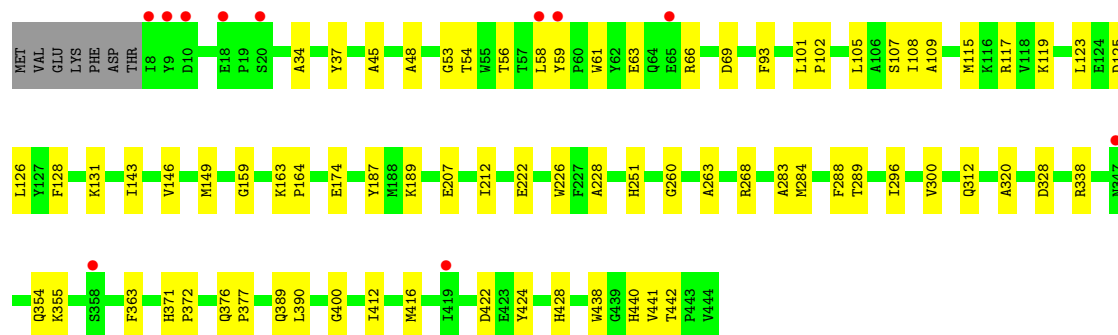
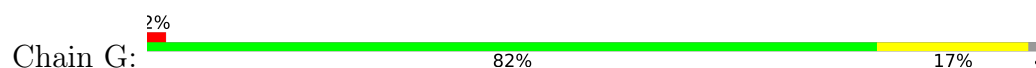
Label	Category
RET	Green
VAL	Green
GLU	Green
LYS	Green
PHE	Green
ASP	Green
THR	Green
I8	Red
Y9	Red
D10	Green
Y11	Yellow
K15	Yellow
P19	Yellow
T38	Yellow
Q41	Yellow
V46	Yellow
A47	Yellow
S51	Yellow
T54	Red
W55	Green
T56	Green
T57	Green
L58	Red
Y59	Red
P60	Yellow
W61	Yellow
Y62	Yellow
L70	Yellow
K73	Green
A74	Green
Y75	Yellow
D79	Yellow
P80	Green
G81	Yellow
W85	Yellow
F93	Yellow
H94	Green
A95	Yellow
F96	Yellow
L104	Yellow
S107	Yellow
I108	Orange
A109	Yellow
M115	Yellow
R122	Yellow
F128	Yellow
E144	Yellow
G145	Green
V146	Yellow
G159	Yellow
K163	Yellow
P164	Yellow
E171	Yellow
Y187	Yellow
M188	Green
K189	Yellow
A206	Yellow
E207	Green
I208	Yellow
M209	Yellow
A210	Yellow
K211	Yellow
L212	Yellow
W226	Yellow
L230	Yellow
L234	Yellow
L235	Yellow
E236	Green
M237	Yellow
E238	Green
Q239	Yellow
G260	Green
A263	Yellow
R282	Yellow
A283	Yellow
M284	Yellow
H285	Yellow
Q312	Yellow
A320	Yellow
D328	Yellow
Q332	Yellow
L336	Yellow
S340	Red
H341	Green
V345	Yellow
K343	Yellow
N347	Yellow
Q354	Yellow
S358	Yellow
L359	Green
K360	Yellow
F363	Yellow
S367	Yellow
H371	Yellow
P372	Yellow
Q376	Yellow
P377	Yellow
V378	Green
L379	Yellow
E380	Red
G383	Yellow
Q389	Yellow
L390	Yellow
H397	Yellow
P398	Yellow
L412	Yellow
L415	Yellow
M416	Yellow
L421	Red
D422	Yellow
E423	Green
Y424	Yellow
H428	Yellow
H440	Yellow
V441	Green
T442	Yellow
P443	Green
V444	Green

Chain E:

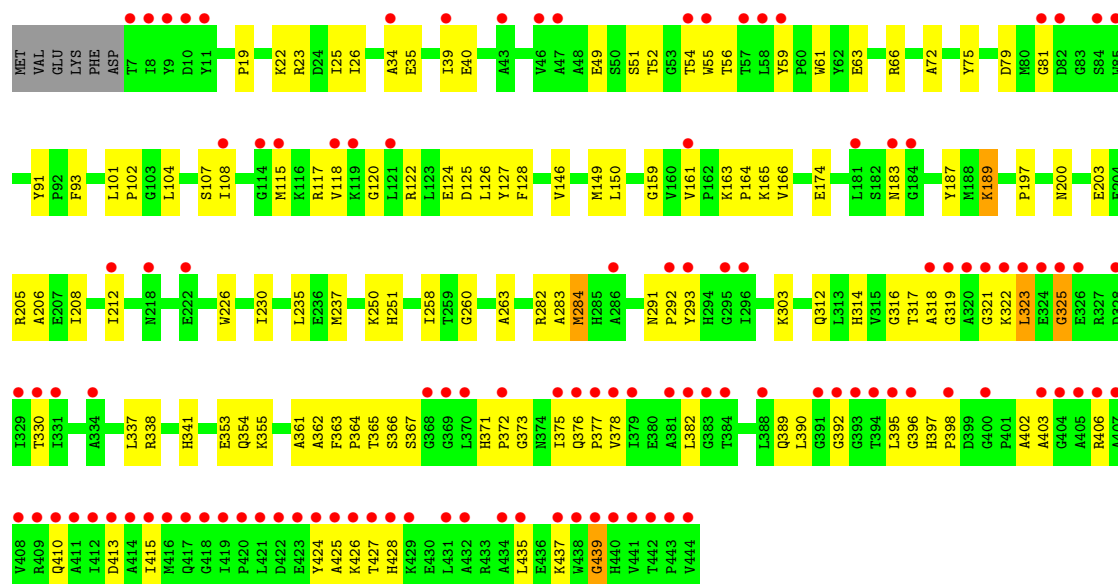
Chain F: 5% 77% 20%



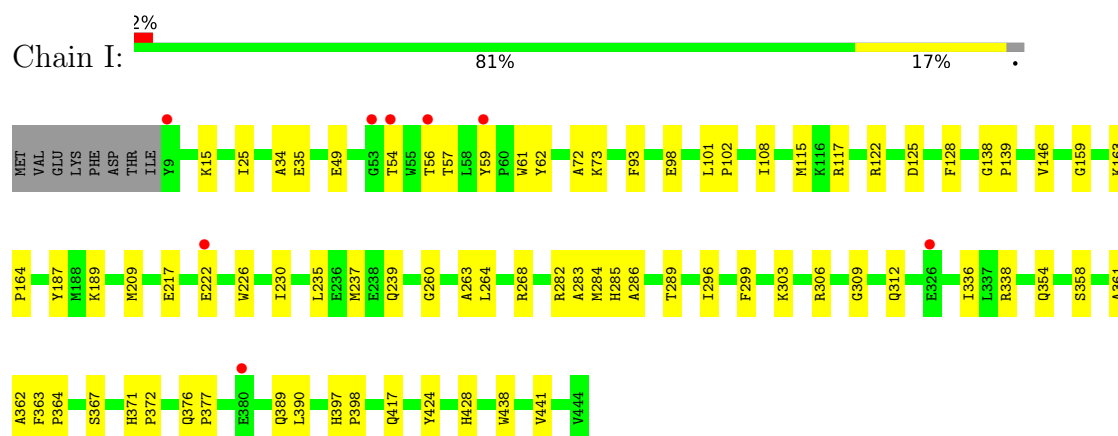
• Molecule 1: Ribulose biphosphate carboxylase



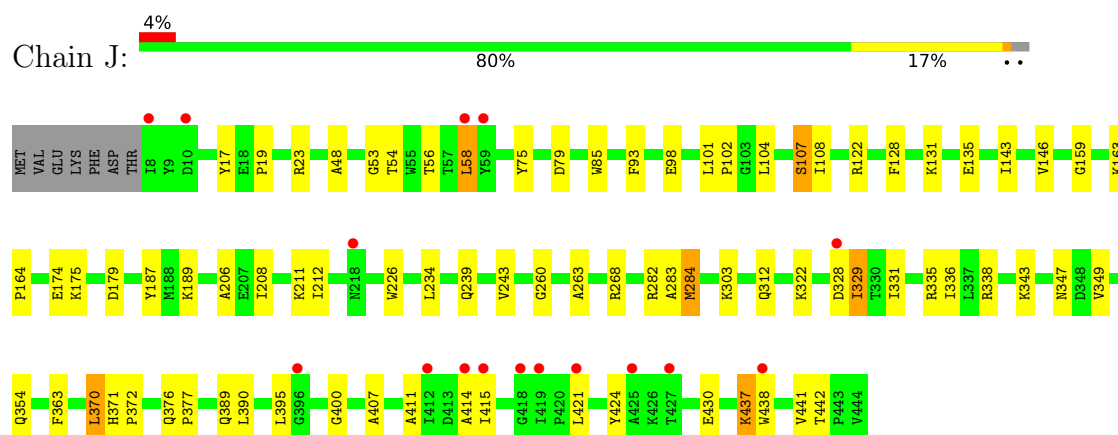
• Molecule 1: Ribulose biphosphate carboxylase



● Molecule 1: Ribulose biphosphate carboxylase



● Molecule 1: Ribulose biphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.47Å 246.24Å 133.08Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	42.86 – 2.09 42.86 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.86-2.09) 96.5 (42.86-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.213 , 0.253 (Not available) , 0.238	Depositor DCC
R_{free} test set	17388 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	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	0.94	EDS
Total number of atoms	36999	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

5.1 Standard geometry

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	0.31	0/3421	0.70	2/4652 (0.0%)
1	B	0.34	0/3505	0.68	2/4753 (0.0%)
1	C	0.35	0/3492	0.69	2/4740 (0.0%)
1	D	0.35	0/3496	0.69	0/4744
1	E	0.33	0/3503	0.68	3/4753 (0.1%)
1	F	0.33	0/3478	0.70	0/4719
1	G	0.33	0/3508	0.69	2/4757 (0.0%)
1	H	0.32	0/3471	0.68	0/4713
1	I	0.33	0/3496	0.67	0/4742
1	J	0.35	0/3503	0.68	2/4753 (0.0%)
All	All	0.33	0/34873	0.69	13/47326 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	GLY	CA-C-N	6.70	126.21	119.24
1	B	400	GLY	C-N-CA	6.70	126.21	119.24
1	A	400	GLY	CA-C-N	5.95	125.42	119.24
1	A	400	GLY	C-N-CA	5.95	125.42	119.24
1	C	400	GLY	CA-C-N	5.93	125.41	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3204	212	0
1	B	3430	0	3346	71	0
1	C	3417	0	3325	80	0
1	D	3421	0	3329	76	0
1	E	3428	0	3319	81	0
1	F	3404	0	3312	73	0
1	G	3433	0	3355	61	0
1	H	3396	0	3282	126	0
1	I	3421	0	3333	60	0
1	J	3428	0	3335	84	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	21	0	7	3	0
3	B	21	0	7	0	0
3	C	21	0	8	1	0
3	D	21	0	8	0	0
3	E	21	0	7	0	0
3	F	21	0	8	0	0
3	G	21	0	8	0	0
3	H	21	0	8	1	0
3	I	21	0	7	0	0
3	J	21	0	7	1	0
4	A	173	0	0	9	0
4	B	290	0	0	6	0
4	C	311	0	0	7	0
4	D	308	0	0	6	0
4	E	258	0	0	8	0
4	F	268	0	0	10	0
4	G	267	0	0	4	0
4	H	185	0	0	10	0
4	I	291	0	0	8	0
4	J	301	0	0	9	0
All	All	36999	0	33215	886	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 13.

The worst 5 of 886 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:A:149:MET:HE3	1:A:250:LYS:CD	1.59	1.29
1:A:38:THR:HG23	1:A:41:GLN:OE1	1.53	1.07
1:G:45:ALA:HB1	1:G:115:MET:HE1	1.36	1.05
1:E:45:ALA:HB1	1:E:115:MET:HE1	1.35	1.04
1:A:149:MET:HE3	1:A:250:LYS:HD2	1.09	1.03

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	434/444 (98%)	394 (91%)	37 (8%)	3 (1%)	18	15
1	B	434/444 (98%)	418 (96%)	16 (4%)	0	100	100
1	C	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	D	434/444 (98%)	422 (97%)	12 (3%)	0	100	100
1	E	435/444 (98%)	418 (96%)	16 (4%)	1 (0%)	43	44
1	F	434/444 (98%)	419 (96%)	14 (3%)	1 (0%)	43	44
1	G	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	H	435/444 (98%)	399 (92%)	32 (7%)	4 (1%)	14	10
1	I	433/444 (98%)	418 (96%)	15 (4%)	0	100	100
1	J	434/444 (98%)	420 (97%)	13 (3%)	1 (0%)	43	44
All	All	4341/4440 (98%)	4146 (96%)	185 (4%)	10 (0%)	43	44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	LYS
1	E	284	MET
1	J	284	MET
1	A	117	ARG
1	A	325	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/356 (91%)	318 (98%)	5 (2%)	57	65
1	B	341/356 (96%)	337 (99%)	4 (1%)	63	72
1	C	338/356 (95%)	333 (98%)	5 (2%)	57	65
1	D	339/356 (95%)	333 (98%)	6 (2%)	51	60
1	E	339/356 (95%)	334 (98%)	5 (2%)	57	65
1	F	335/356 (94%)	327 (98%)	8 (2%)	43	49
1	G	342/356 (96%)	338 (99%)	4 (1%)	63	72
1	H	330/356 (93%)	326 (99%)	4 (1%)	63	72
1	I	340/356 (96%)	339 (100%)	1 (0%)	86	91
1	J	341/356 (96%)	334 (98%)	7 (2%)	47	54
All	All	3368/3560 (95%)	3319 (98%)	49 (2%)	57	65

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	181	LEU
1	G	328	ASP
1	F	235	LEU
1	F	363	PHE
1	H	107	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	312	GLN
1	I	312	GLN
1	G	354	GLN
1	H	78	HIS
1	I	376	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	F	189	2,1	10,11,12	0.99	0	6,12,14	1.37	1 (16%)
1	KCX	J	189	2,1	10,11,12	0.90	0	6,12,14	1.36	1 (16%)
1	KCX	E	189	2,1	10,11,12	0.91	0	6,12,14	1.41	1 (16%)
1	KCX	B	189	2,1	10,11,12	0.95	0	6,12,14	1.18	1 (16%)
1	KCX	G	189	2,1	10,11,12	0.97	0	6,12,14	1.35	1 (16%)
1	KCX	A	189	2,1	10,11,12	0.93	0	6,12,14	1.30	1 (16%)
1	KCX	C	189	2,1	10,11,12	0.93	0	6,12,14	1.14	1 (16%)
1	KCX	H	189	2,1	10,11,12	0.87	0	6,12,14	1.29	1 (16%)
1	KCX	D	189	2,1	10,11,12	0.91	0	6,12,14	1.45	1 (16%)
1	KCX	I	189	2,1	10,11,12	0.99	0	6,12,14	1.35	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	F	189	2,1	-	1/9/10/12	-
1	KCX	J	189	2,1	-	0/9/10/12	-
1	KCX	E	189	2,1	-	0/9/10/12	-
1	KCX	B	189	2,1	-	0/9/10/12	-
1	KCX	G	189	2,1	-	0/9/10/12	-
1	KCX	A	189	2,1	-	0/9/10/12	-
1	KCX	C	189	2,1	-	1/9/10/12	-
1	KCX	H	189	2,1	-	1/9/10/12	-
1	KCX	D	189	2,1	-	1/9/10/12	-
1	KCX	I	189	2,1	-	0/9/10/12	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	KCX	OQ1-CX-NZ	-3.45	119.67	124.92
1	F	189	KCX	OQ1-CX-NZ	-3.23	120.02	124.92
1	G	189	KCX	OQ1-CX-NZ	-3.21	120.05	124.92
1	E	189	KCX	OQ1-CX-NZ	-3.20	120.06	124.92
1	J	189	KCX	OQ1-CX-NZ	-3.17	120.10	124.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	189	KCX	C-CA-CB-CG
1	D	189	KCX	C-CA-CB-CG
1	F	189	KCX	C-CA-CB-CG
1	H	189	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	189	KCX	1	0
1	C	189	KCX	1	0
1	H	189	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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$
3	CAP	A	600	2	18,20,20	0.97	0	23,31,31	1.04	1 (4%)
3	CAP	I	600	2	18,20,20	0.88	0	23,31,31	0.93	1 (4%)
3	CAP	J	600	2	18,20,20	0.99	0	23,31,31	0.98	1 (4%)
3	CAP	F	600	2	18,20,20	0.89	0	23,31,31	0.95	1 (4%)
3	CAP	H	600	2	18,20,20	0.89	0	23,31,31	1.06	1 (4%)
3	CAP	D	600	2	18,20,20	0.88	0	23,31,31	1.01	1 (4%)
3	CAP	B	600	2	18,20,20	0.91	0	23,31,31	1.04	1 (4%)
3	CAP	C	600	2	18,20,20	0.94	0	23,31,31	0.96	1 (4%)
3	CAP	G	600	2	18,20,20	0.85	0	23,31,31	1.00	1 (4%)
3	CAP	E	600	2	18,20,20	0.90	0	23,31,31	1.03	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	A	600	2	-	6/29/29/29	-
3	CAP	I	600	2	-	6/29/29/29	-
3	CAP	J	600	2	-	6/29/29/29	-
3	CAP	F	600	2	-	6/29/29/29	-
3	CAP	H	600	2	-	11/29/29/29	-
3	CAP	D	600	2	-	9/29/29/29	-
3	CAP	B	600	2	-	8/29/29/29	-
3	CAP	C	600	2	-	6/29/29/29	-
3	CAP	G	600	2	-	6/29/29/29	-
3	CAP	E	600	2	-	6/29/29/29	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	600	CAP	O7-C-C2	3.65	120.17	114.06
3	A	600	CAP	O7-C-C2	3.30	119.59	114.06
3	B	600	CAP	O7-C-C2	3.30	119.59	114.06
3	G	600	CAP	O7-C-C2	3.29	119.56	114.06
3	D	600	CAP	O7-C-C2	3.28	119.55	114.06

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

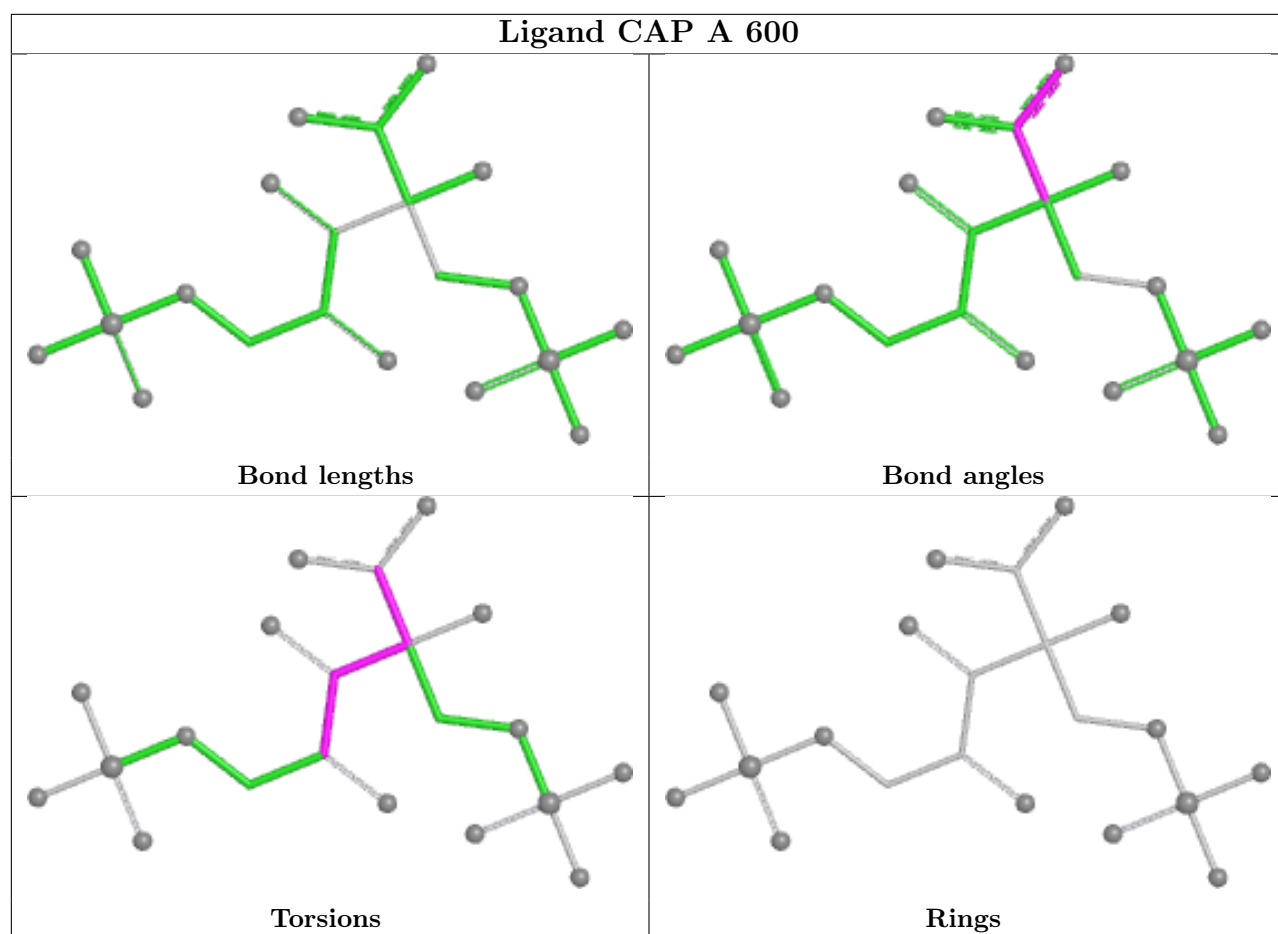
Mol	Chain	Res	Type	Atoms
3	A	600	CAP	O6-C-C2-C1
3	A	600	CAP	O7-C-C2-C1
3	A	600	CAP	O6-C-C2-O2
3	A	600	CAP	O7-C-C2-O2
3	B	600	CAP	O6-C-C2-C1

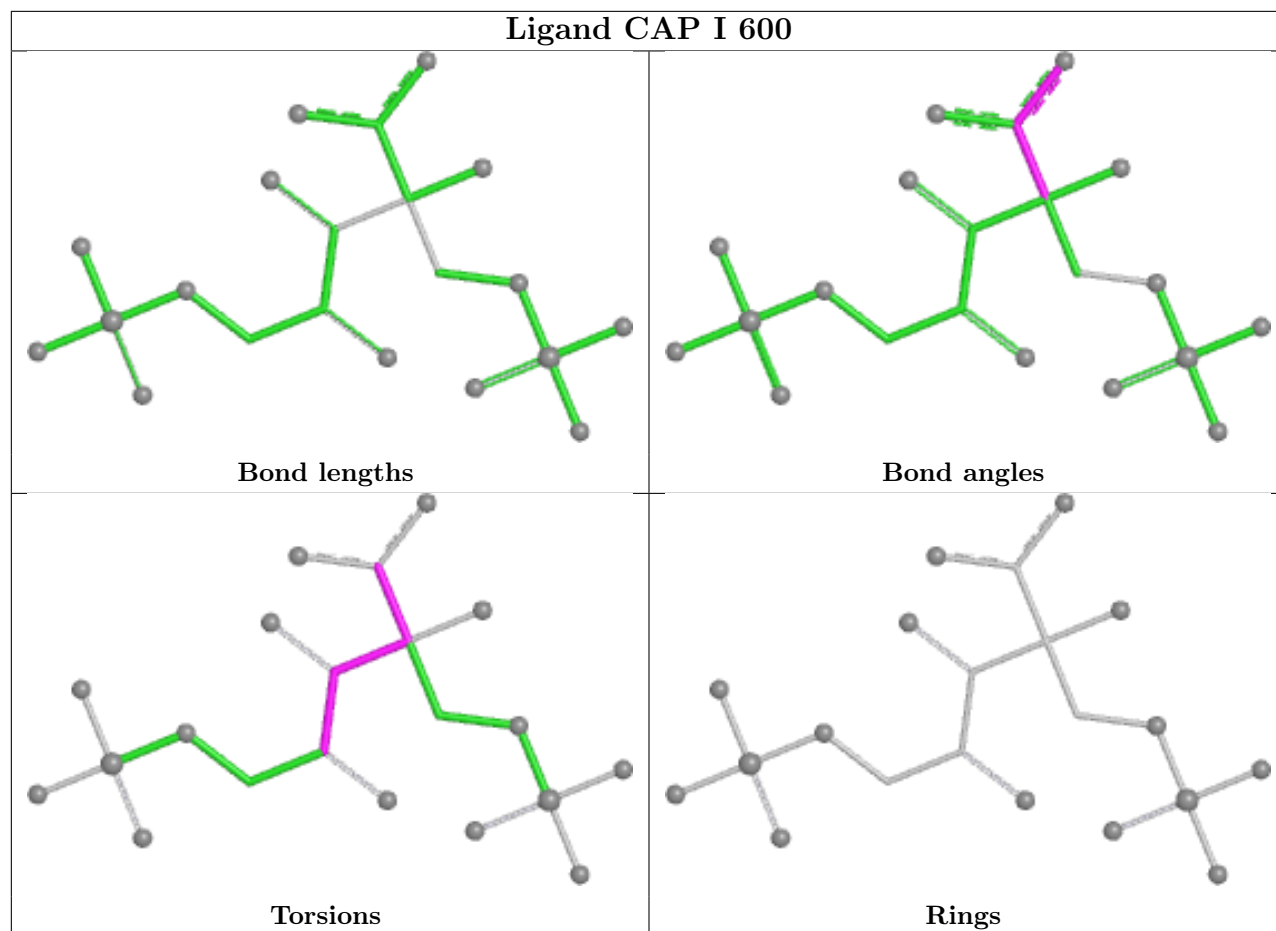
There are no ring outliers.

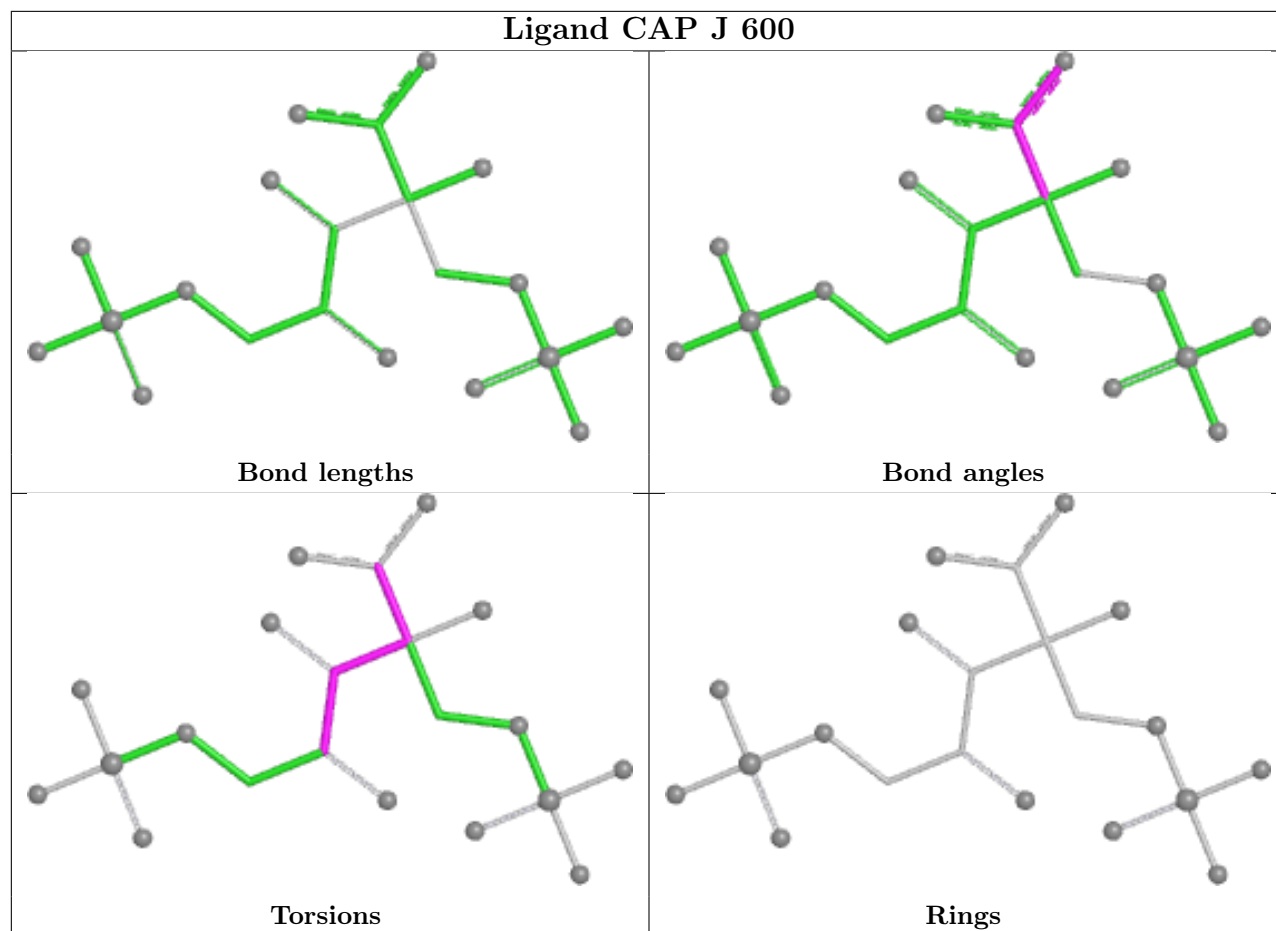
4 monomers are involved in 6 short contacts:

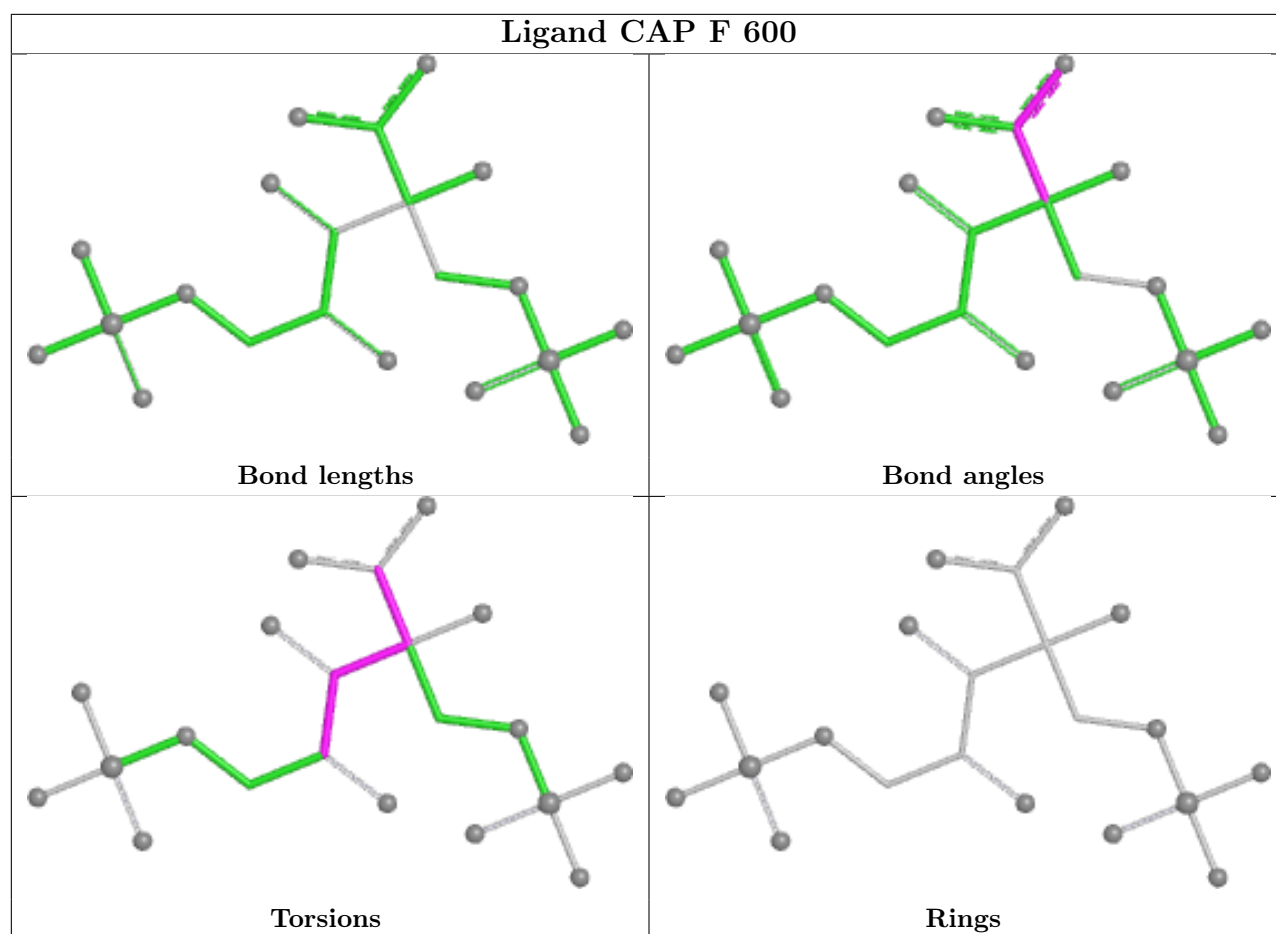
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	CAP	3	0
3	J	600	CAP	1	0
3	H	600	CAP	1	0
3	C	600	CAP	1	0

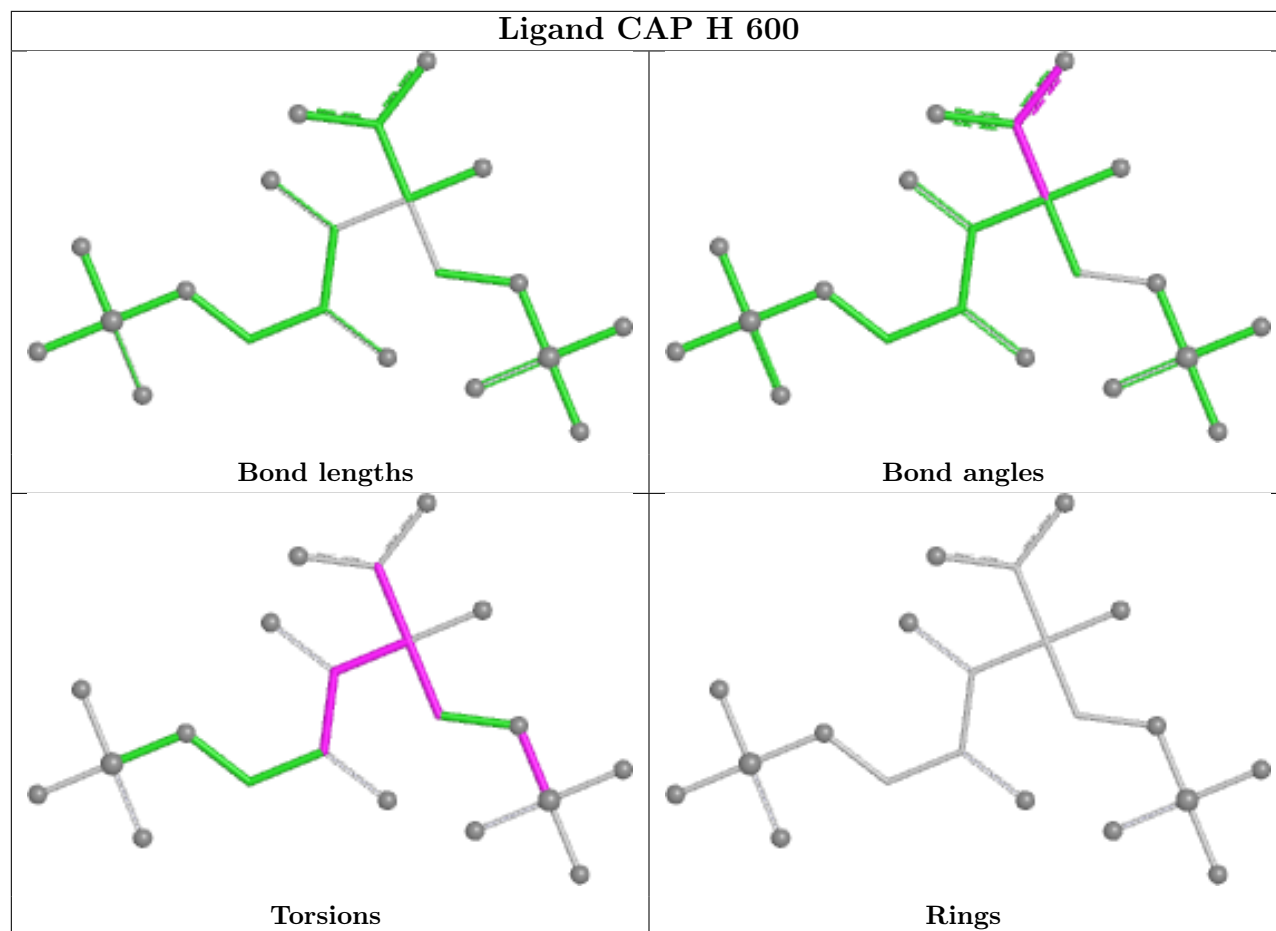
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

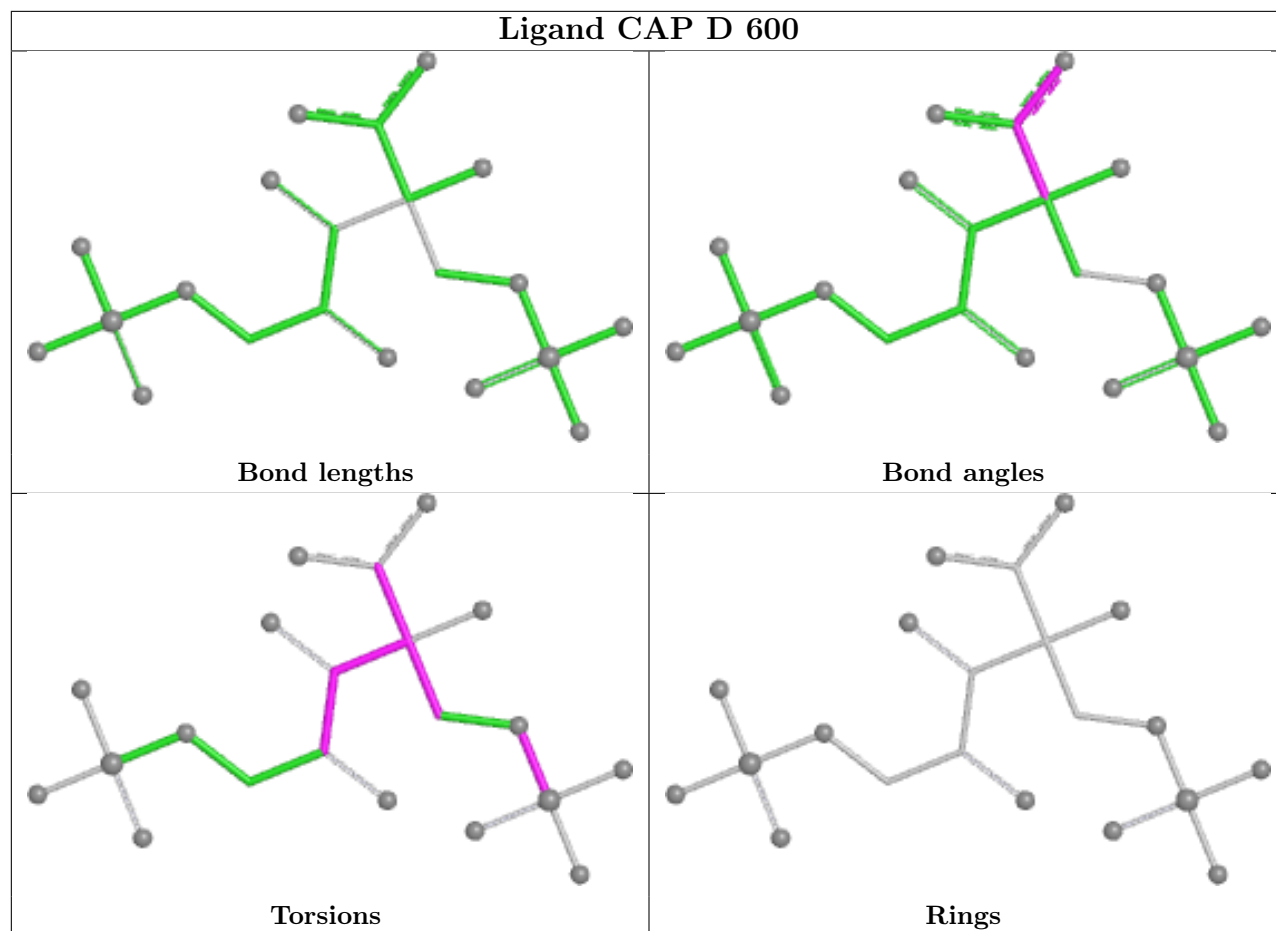


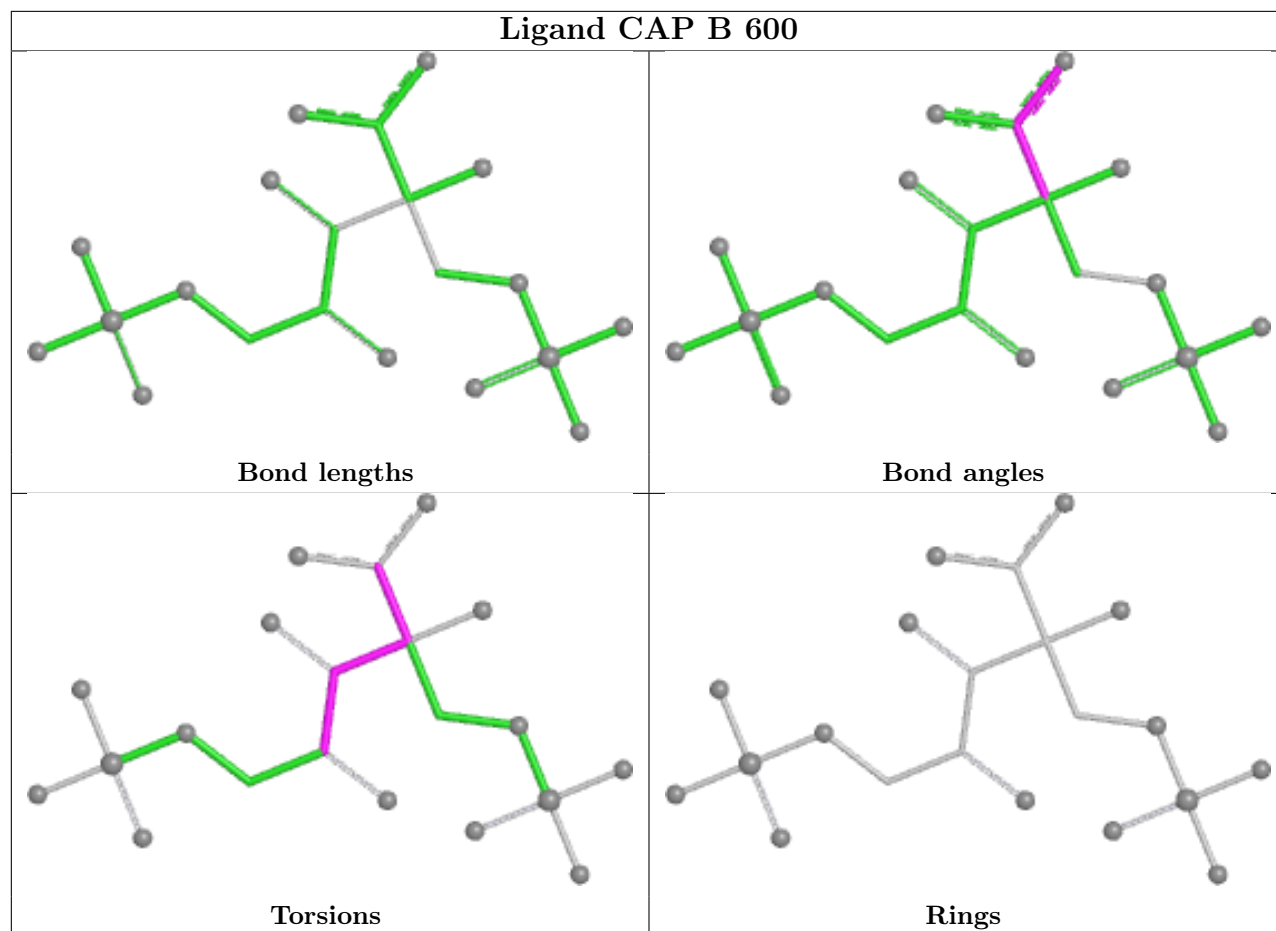


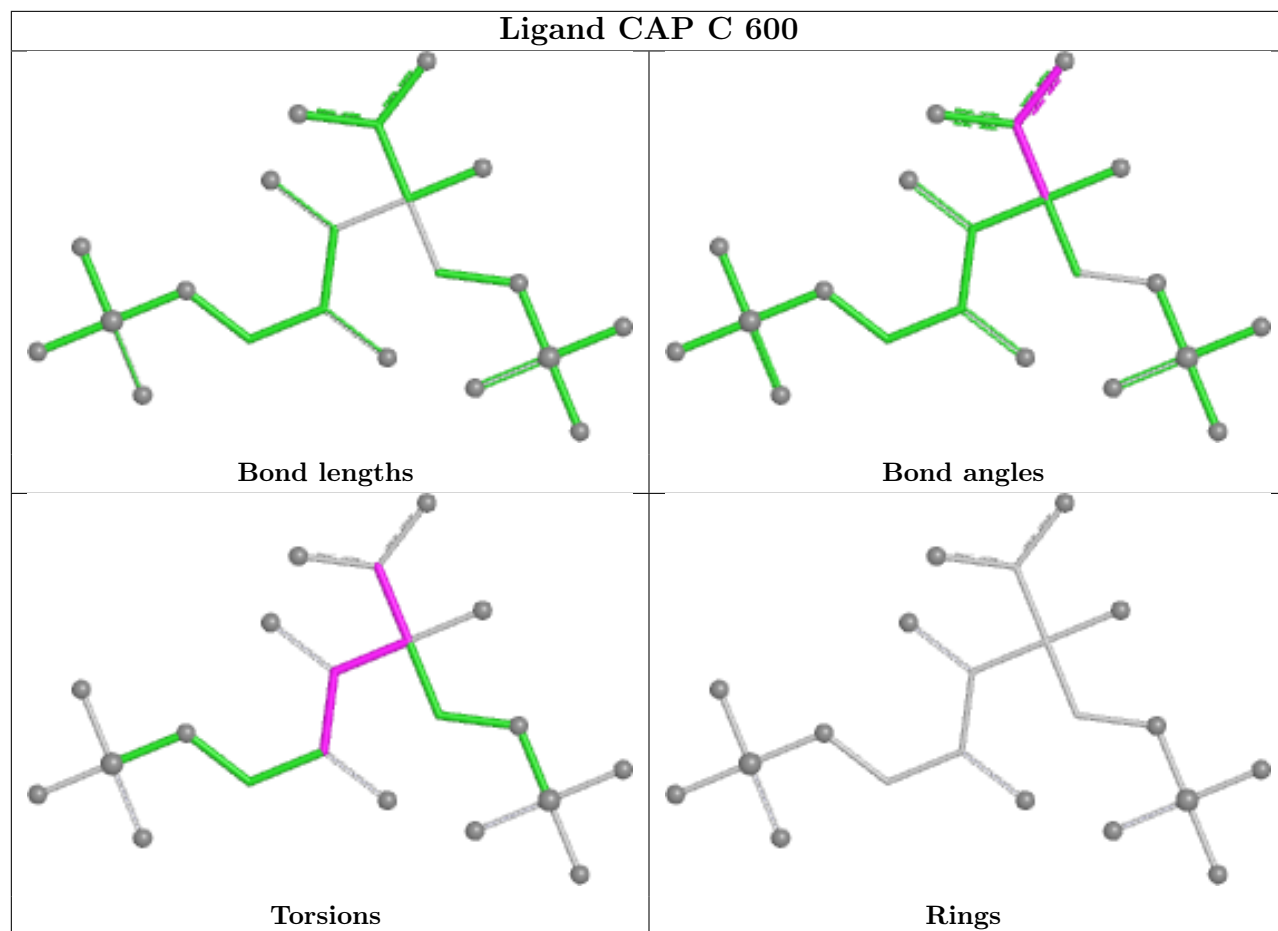


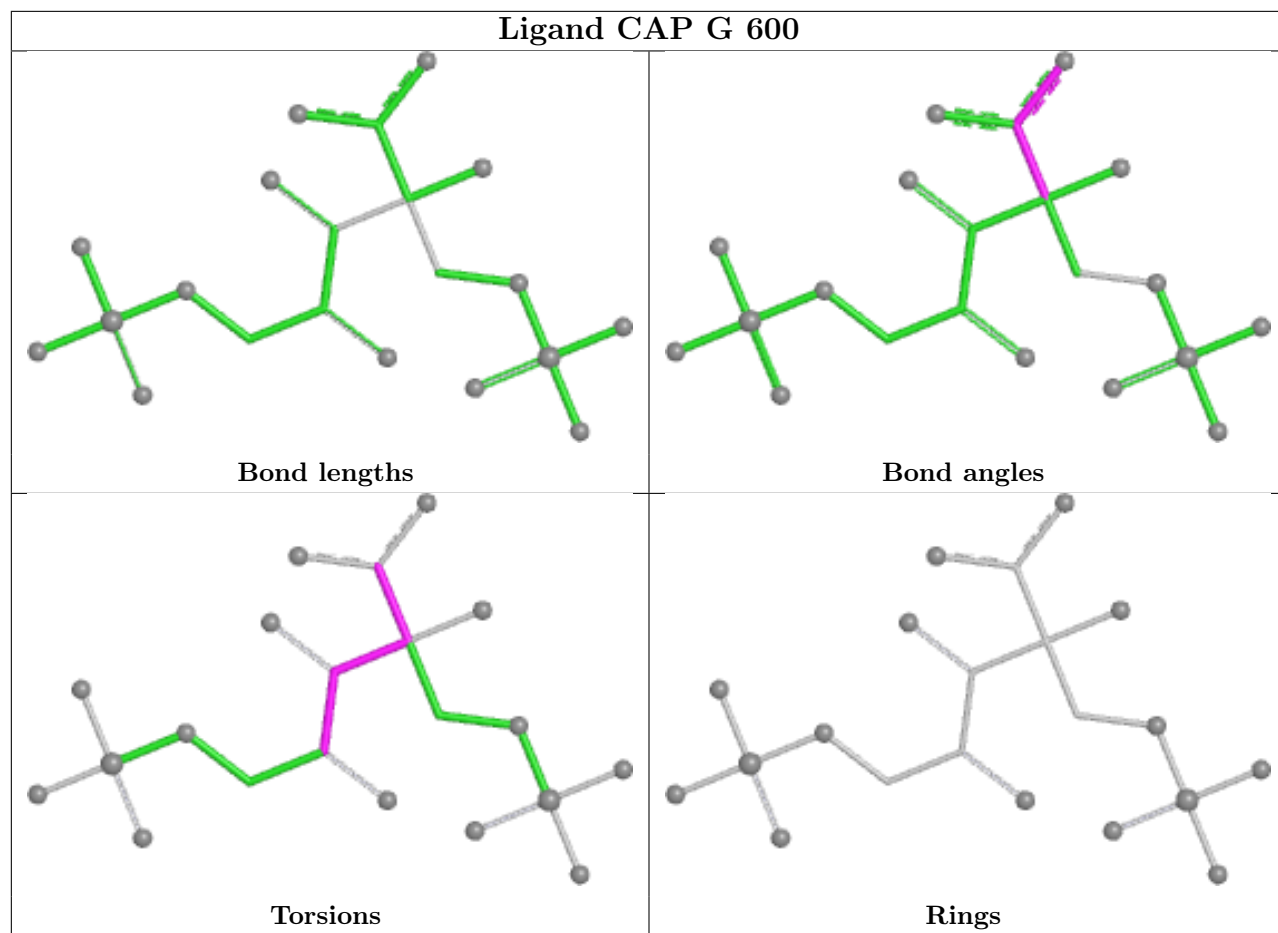


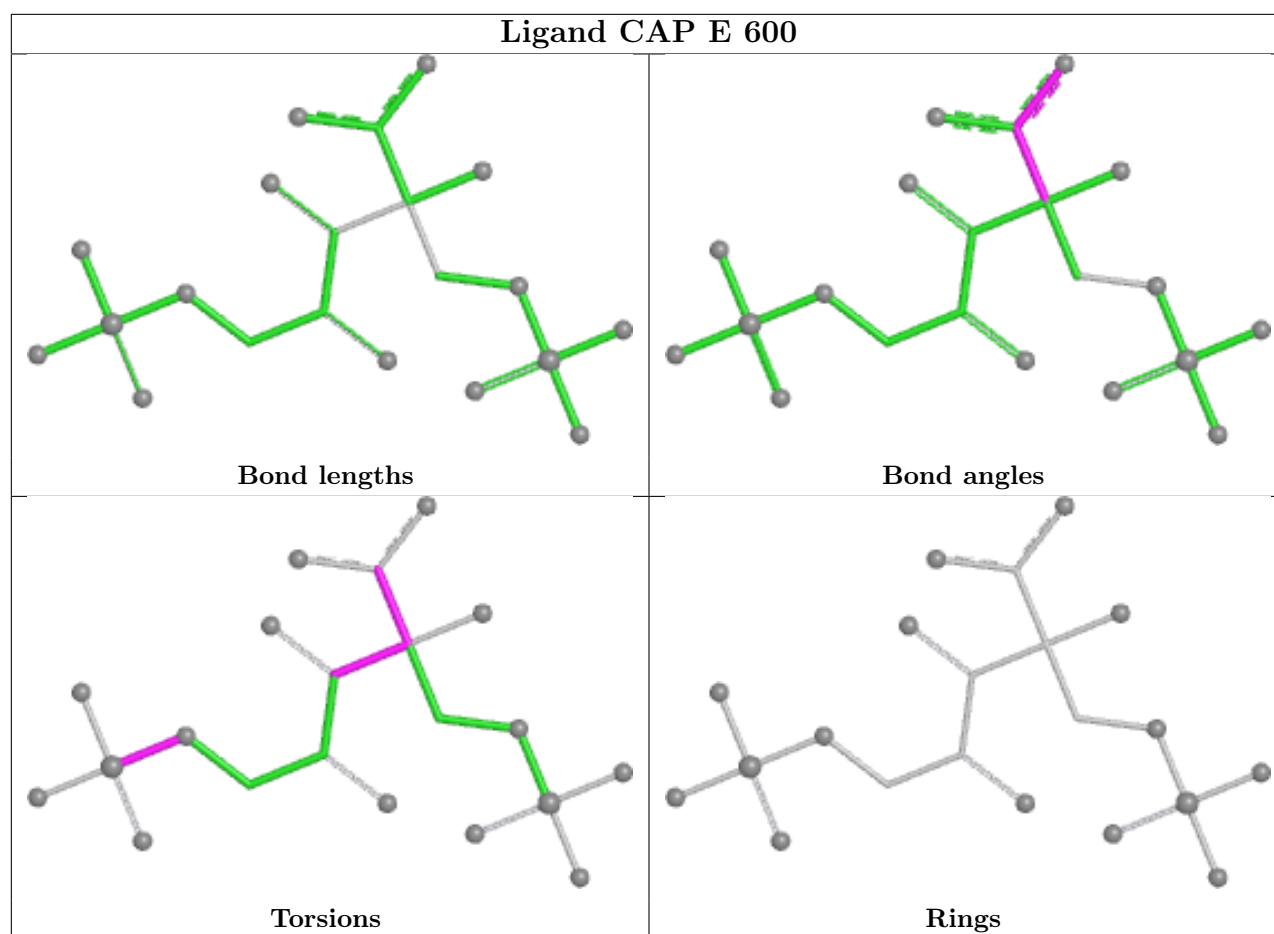












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/444 (98%)	1.80	187 (42%) 0 1	22, 36, 52, 58	0
1	B	436/444 (98%)	0.11	6 (1%) 73 75	13, 22, 34, 37	0
1	C	436/444 (98%)	0.19	15 (3%) 48 50	12, 21, 40, 45	0
1	D	436/444 (98%)	0.06	8 (1%) 67 70	11, 20, 32, 39	0
1	E	437/444 (98%)	0.32	29 (6%) 24 26	15, 24, 47, 51	0
1	F	436/444 (98%)	0.35	23 (5%) 32 34	12, 24, 38, 46	0
1	G	436/444 (98%)	0.18	11 (2%) 58 61	13, 24, 36, 41	0
1	H	437/444 (98%)	1.26	112 (25%) 1 2	22, 32, 57, 61	0
1	I	435/444 (97%)	0.04	8 (1%) 67 70	15, 23, 34, 40	0
1	J	436/444 (98%)	0.12	16 (3%) 45 47	11, 20, 41, 47	0
All	All	4361/4440 (98%)	0.44	415 (9%) 14 14	11, 24, 42, 61	0

The worst 5 of 415 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	6.9
1	H	443	PRO	6.0
1	A	421	LEU	5.6
1	F	59	TYR	5.5
1	I	59	TYR	5.4

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($\text{\AA}^2$)	Q<0.9
1	KCX	A	189	12/13	0.92	0.11	29,30,31,31	0
1	KCX	H	189	12/13	0.92	0.10	30,30,31,31	0
1	KCX	F	189	12/13	0.95	0.08	17,18,20,20	0
1	KCX	E	189	12/13	0.95	0.07	21,22,23,23	0
1	KCX	C	189	12/13	0.96	0.07	14,16,17,17	0
1	KCX	I	189	12/13	0.96	0.06	17,18,18,18	0
1	KCX	G	189	12/13	0.97	0.05	16,17,17,17	0
1	KCX	B	189	12/13	0.97	0.06	18,19,19,20	0
1	KCX	D	189	12/13	0.97	0.06	11,14,15,15	0
1	KCX	J	189	12/13	0.97	0.06	18,18,19,20	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.

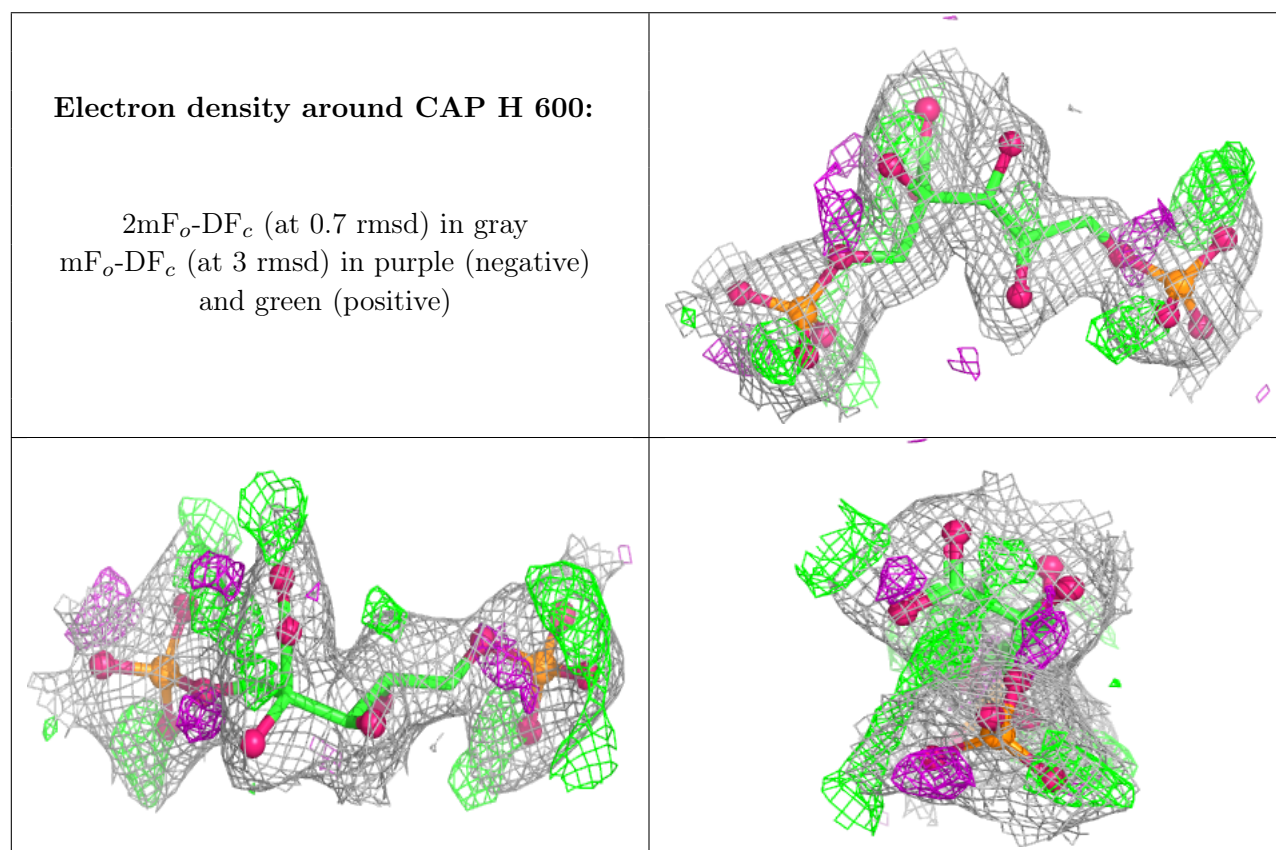
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAP	H	600	21/21	0.87	0.13	31,34,36,37	0
3	CAP	A	600	21/21	0.88	0.13	27,33,34,35	0
2	MG	H	500	1/1	0.96	0.05	29,29,29,29	0
3	CAP	J	600	21/21	0.96	0.08	17,21,22,22	0
3	CAP	C	600	21/21	0.97	0.06	19,21,22,23	0
3	CAP	E	600	21/21	0.97	0.07	21,24,26,26	0
3	CAP	G	600	21/21	0.97	0.06	17,17,18,18	0
2	MG	A	500	1/1	0.97	0.04	29,29,29,29	0
3	CAP	B	600	21/21	0.97	0.06	17,20,21,22	0
3	CAP	F	600	21/21	0.98	0.05	15,17,17,18	0
2	MG	G	500	1/1	0.98	0.05	16,16,16,16	0
3	CAP	D	600	21/21	0.98	0.05	13,14,15,16	0
3	CAP	I	600	21/21	0.98	0.05	16,18,18,19	0
2	MG	C	500	1/1	0.98	0.02	16,16,16,16	0
2	MG	I	500	1/1	0.99	0.02	13,13,13,13	0
2	MG	J	500	1/1	0.99	0.02	16,16,16,16	0
2	MG	E	500	1/1	0.99	0.02	21,21,21,21	0
2	MG	F	500	1/1	0.99	0.02	19,19,19,19	0
2	MG	B	500	1/1	0.99	0.03	18,18,18,18	0

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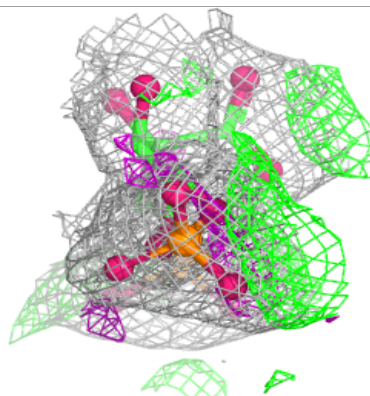
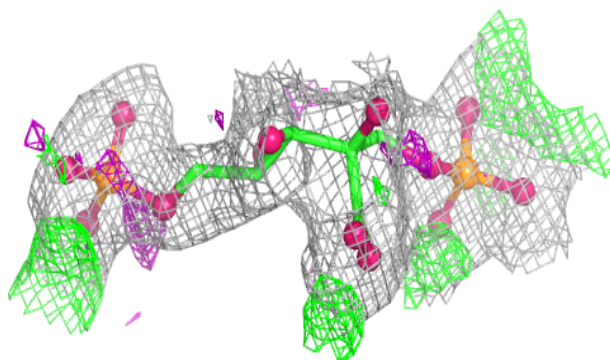
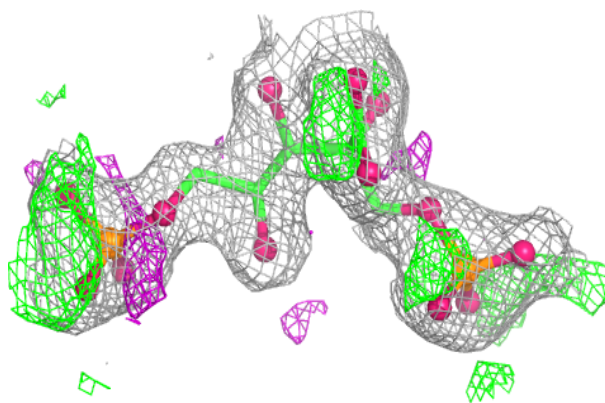
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	500	1/1	0.99	0.02	11,11,11,11	0

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.

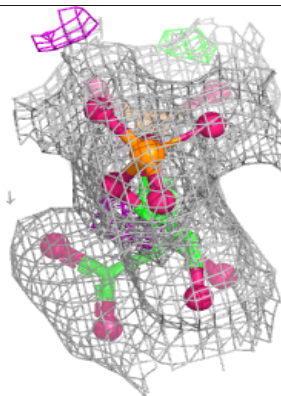
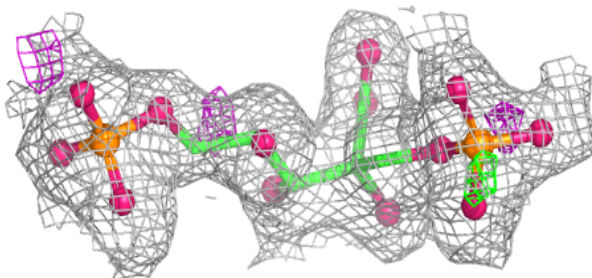
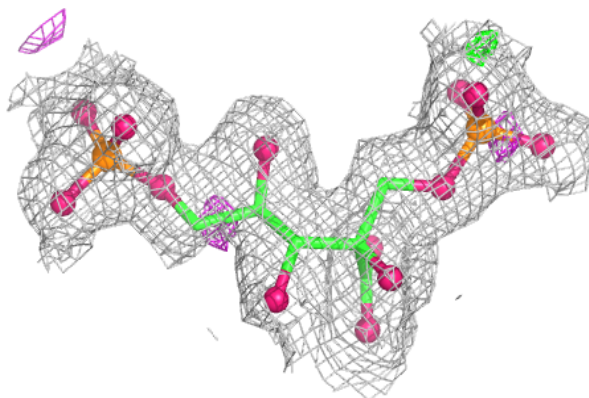


Electron density around CAP A 600:

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

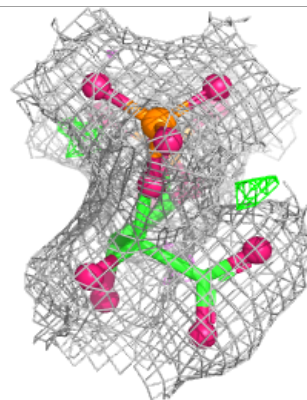
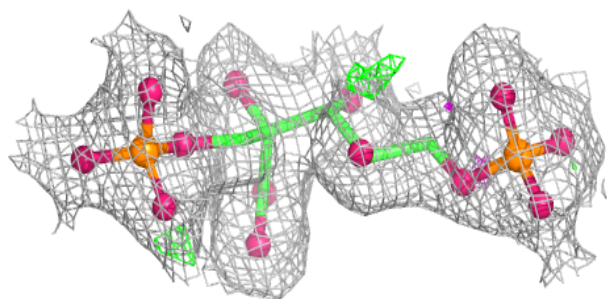
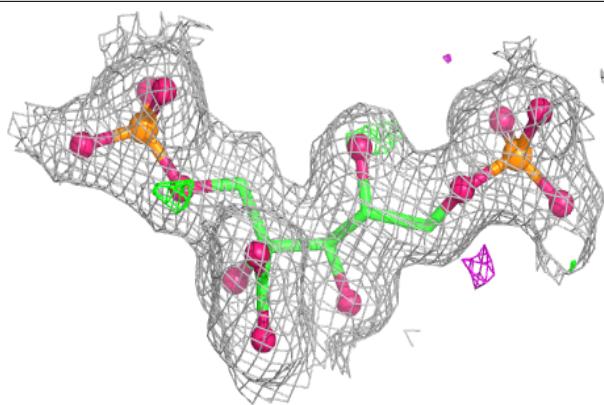
**Electron density around CAP J 600:**

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

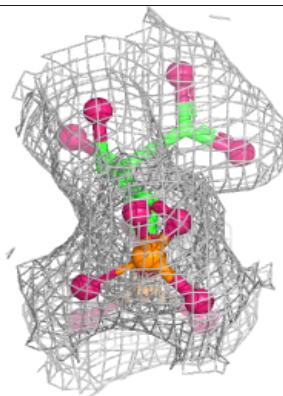
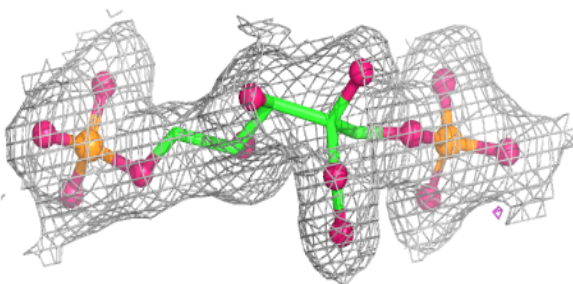
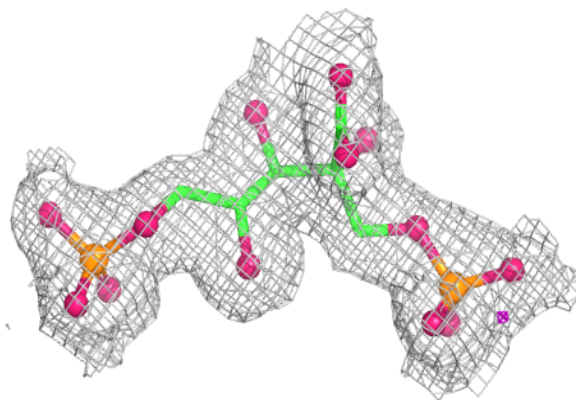


Electron density around CAP C 600:

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

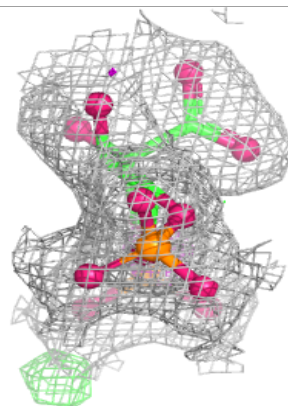
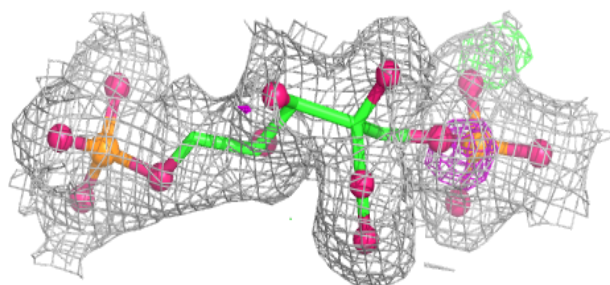
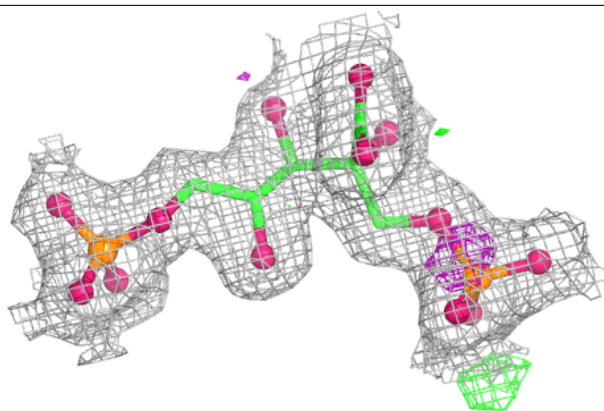
**Electron density around CAP E 600:**

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

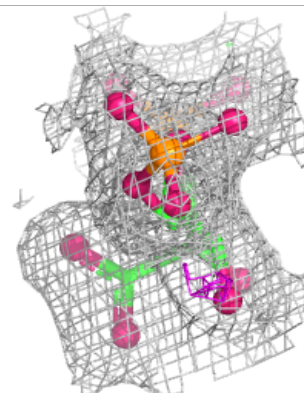
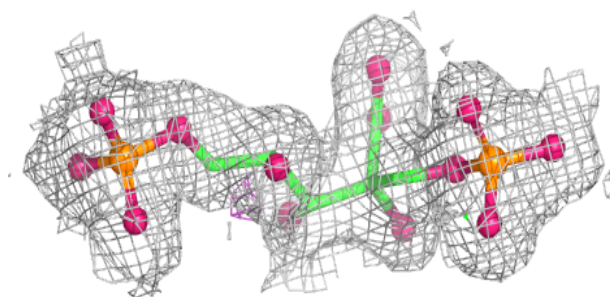
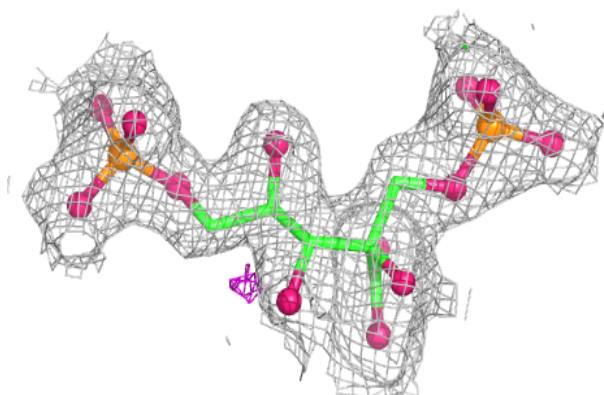


Electron density around CAP G 600:

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

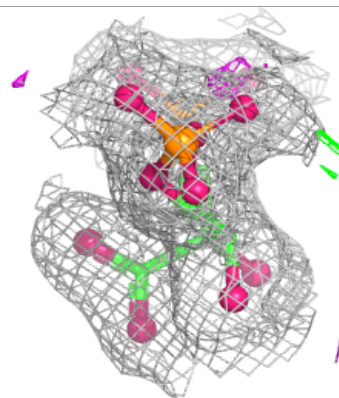
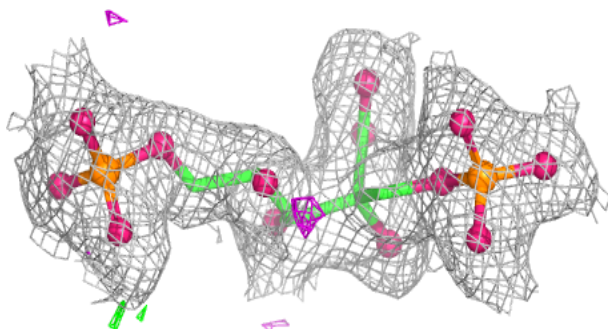
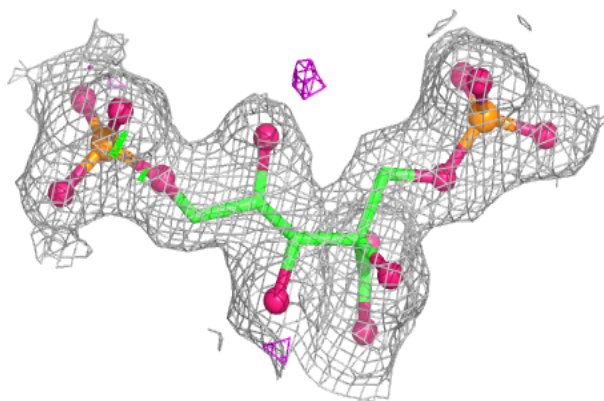
**Electron density around CAP B 600:**

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

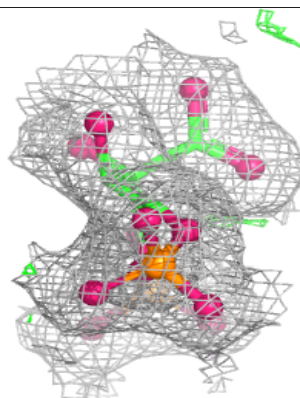
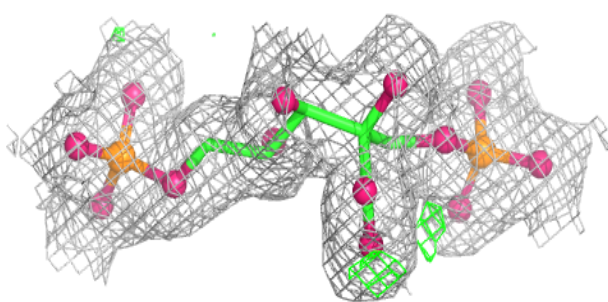
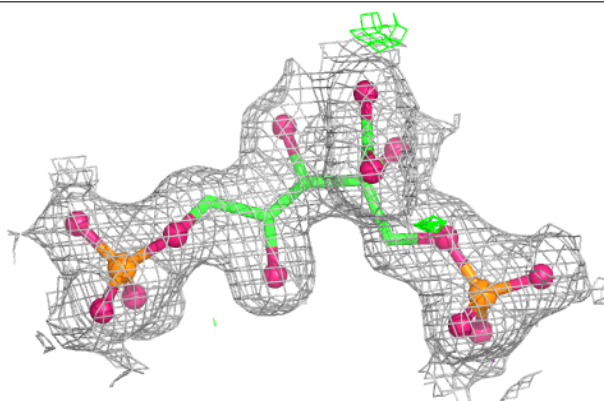


Electron density around CAP F 600:

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

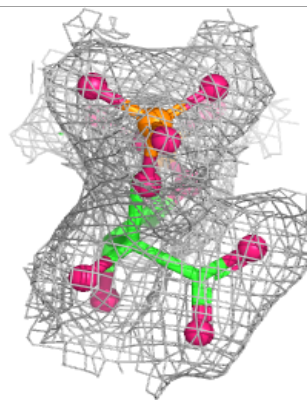
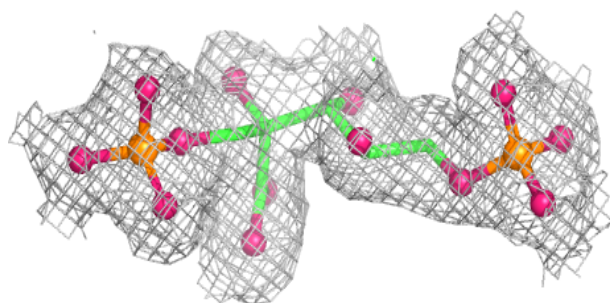
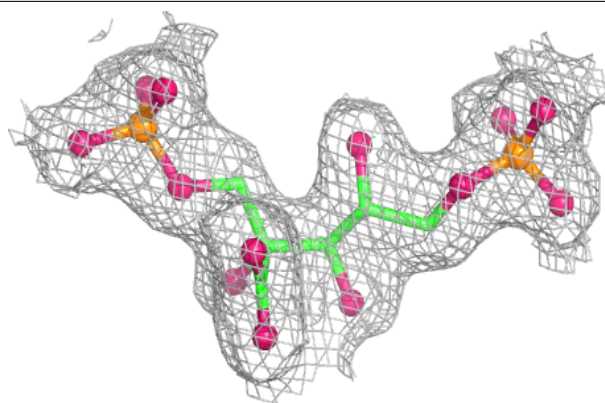
**Electron density around CAP D 600:**

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



Electron density around CAP I 600:

$2mF_o-DF_c$ (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.