Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:09 am BST

PDB ID	:	3WQP
Title	:	Crystal structure of Rubisco T289D mutant from Thermococcus kodakarensis
Authors	:	Fujihashi, M.; Nishitani, Y.; Kiriyama, T.; Miki, K.
Deposited on	:	2014-01-29
Resolution	:	2.25 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

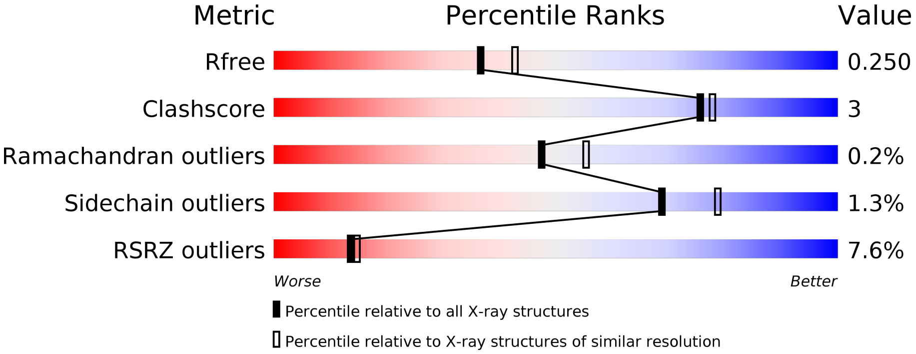
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

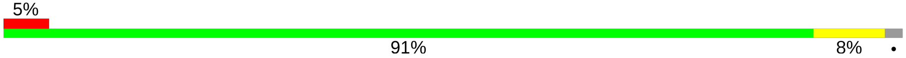
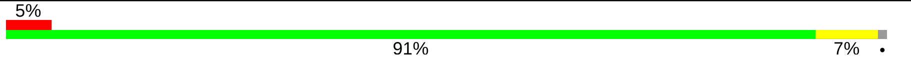
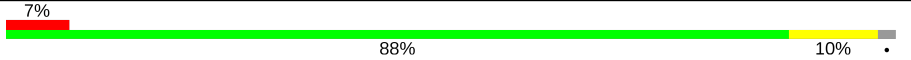
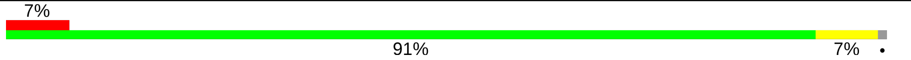
The reported resolution of this entry is 2.25 Å.

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	

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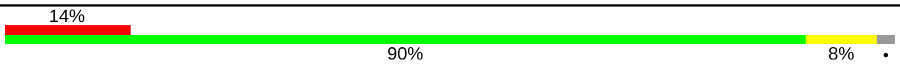
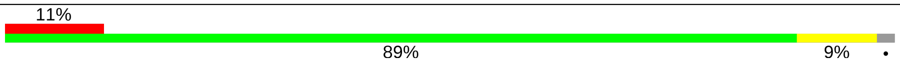
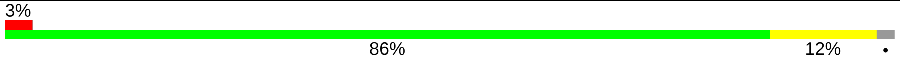
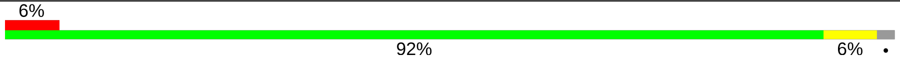
Mol	Chain	Length	Quality of chain
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36577 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	437	Total	C	N	O	S	0	0	0
			3425	2200	584	631	10			
1	B	438	Total	C	N	O	S	0	0	0
			3440	2207	587	636	10			
1	C	438	Total	C	N	O	S	0	0	0
			3443	2209	588	636	10			
1	D	436	Total	C	N	O	S	0	0	0
			3441	2209	587	635	10			
1	E	438	Total	C	N	O	S	0	0	0
			3438	2206	586	636	10			
1	F	436	Total	C	N	O	S	0	0	0
			3408	2185	584	629	10			
1	G	436	Total	C	N	O	S	0	0	0
			3416	2192	581	633	10			
1	H	437	Total	C	N	O	S	0	0	0
			3423	2200	586	627	10			
1	I	436	Total	C	N	O	S	0	0	0
			3434	2204	587	633	10			
1	J	437	Total	C	N	O	S	0	0	0
			3438	2209	586	633	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
B	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
C	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
D	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
E	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
F	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
G	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
H	289	ASP	THR	ENGINEERED MUTATION	UNP O93627
I	289	ASP	THR	ENGINEERED MUTATION	UNP O93627

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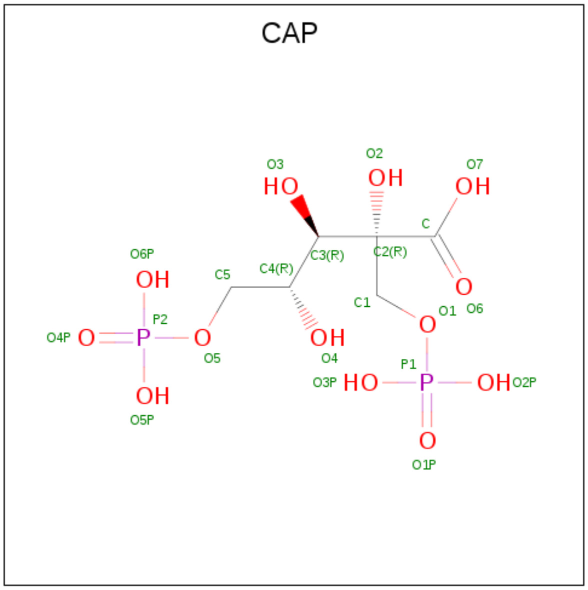
Chain	Residue	Modelled	Actual	Comment	Reference
J	289	ASP	THR	ENGINEERED MUTATION	UNP O93627

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

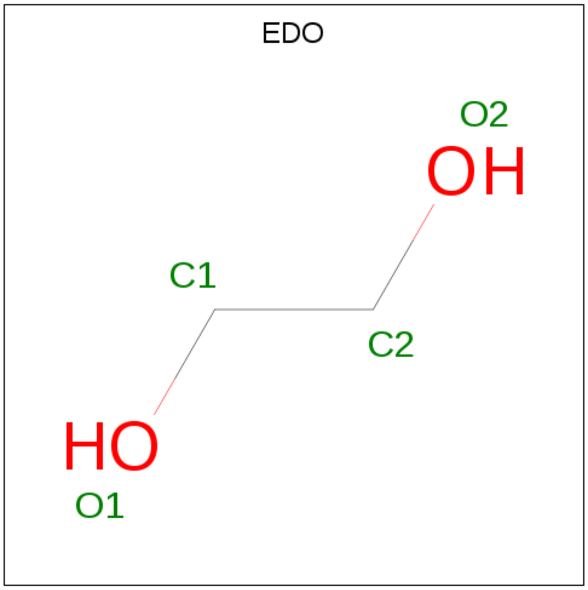
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	183	Total O 183 183	0	0
5	B	127	Total O 127 127	0	0

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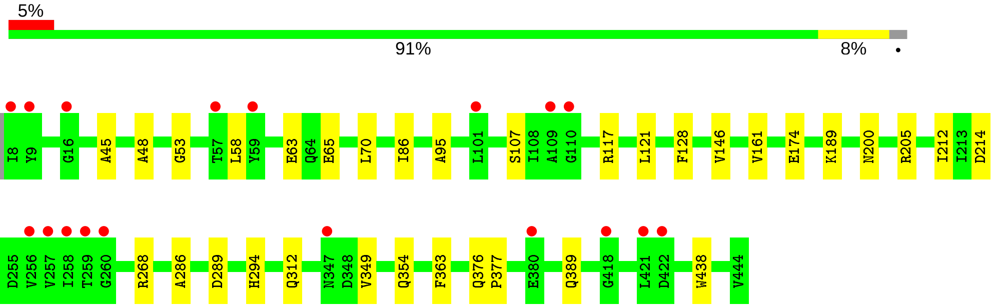
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	223	Total O 223 223	0	0
5	D	240	Total O 240 240	0	0
5	E	252	Total O 252 252	0	0
5	F	170	Total O 170 170	0	0
5	G	133	Total O 133 133	0	0
5	H	184	Total O 184 184	0	0
5	I	244	Total O 244 244	0	0
5	J	255	Total O 255 255	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.

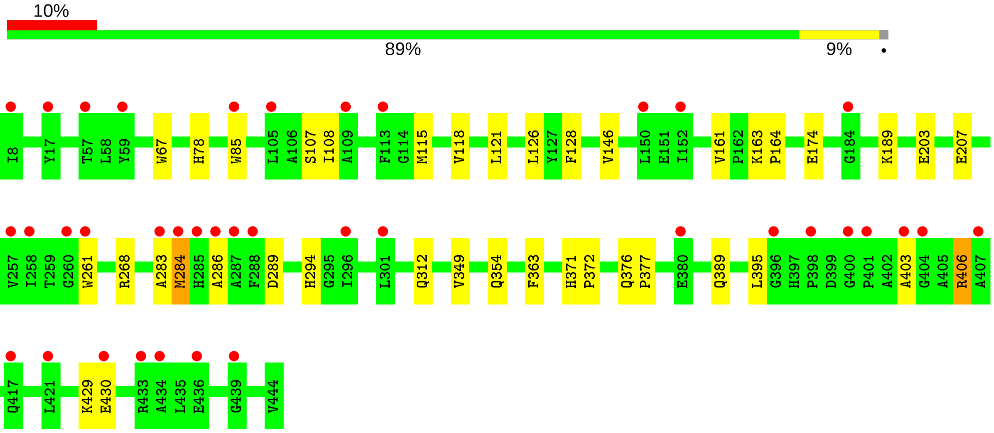
- Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



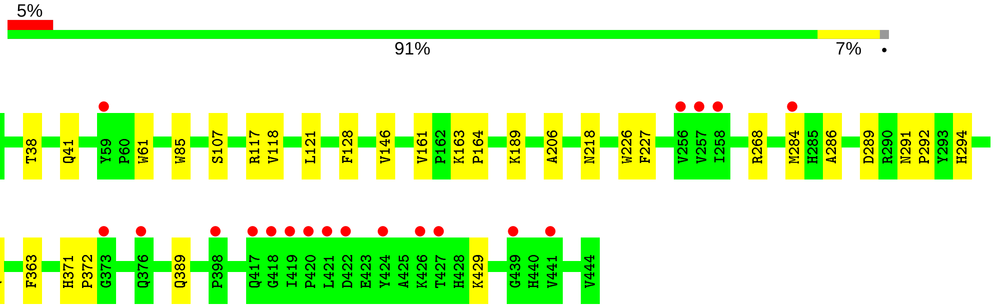
- Molecule 1: Ribulose bisphosphate carboxylase

Chain B:



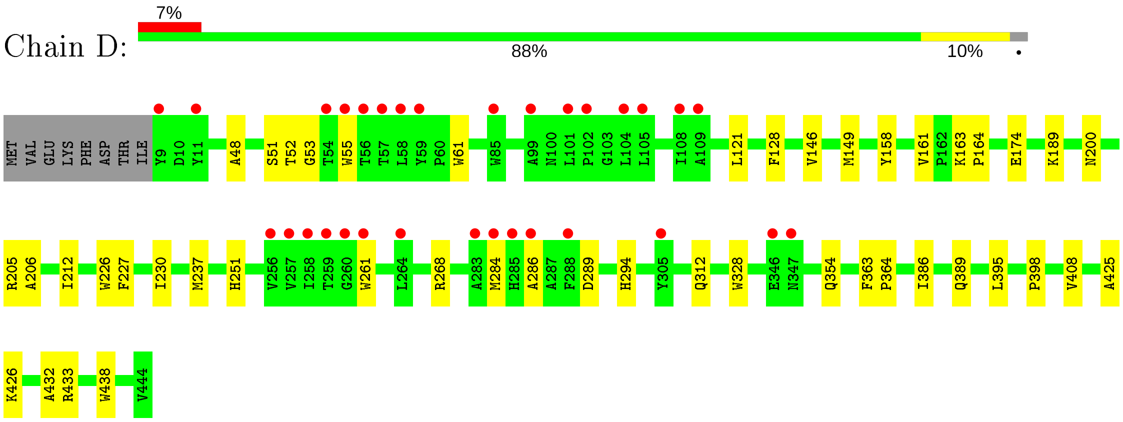
- Molecule 1: Ribulose bisphosphate carboxylase

Chain C:



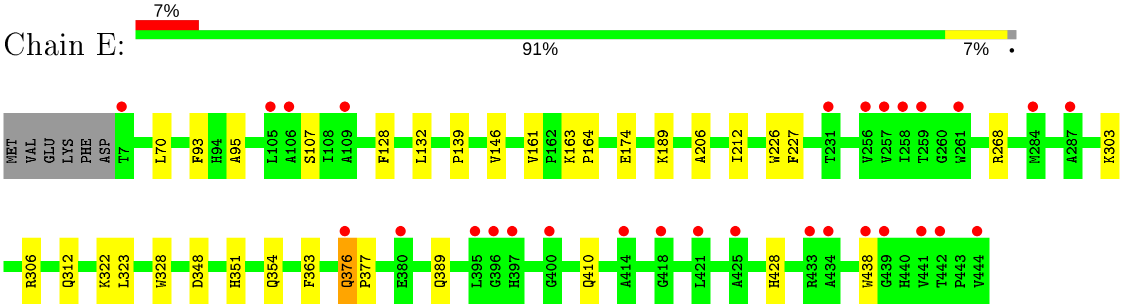
- Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



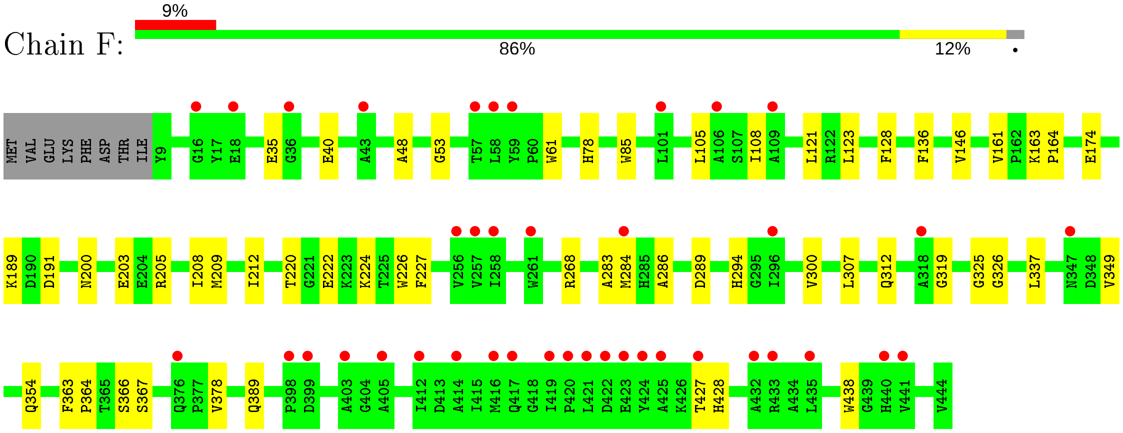
- Molecule 1: Ribulose bisphosphate carboxylase

Chain E:



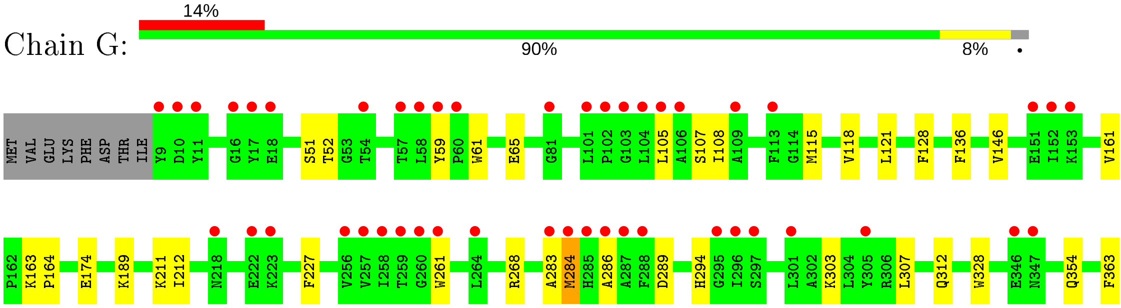
- Molecule 1: Ribulose bisphosphate carboxylase

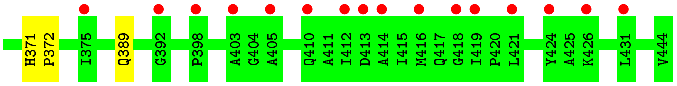
Chain F:



- Molecule 1: Ribulose bisphosphate carboxylase

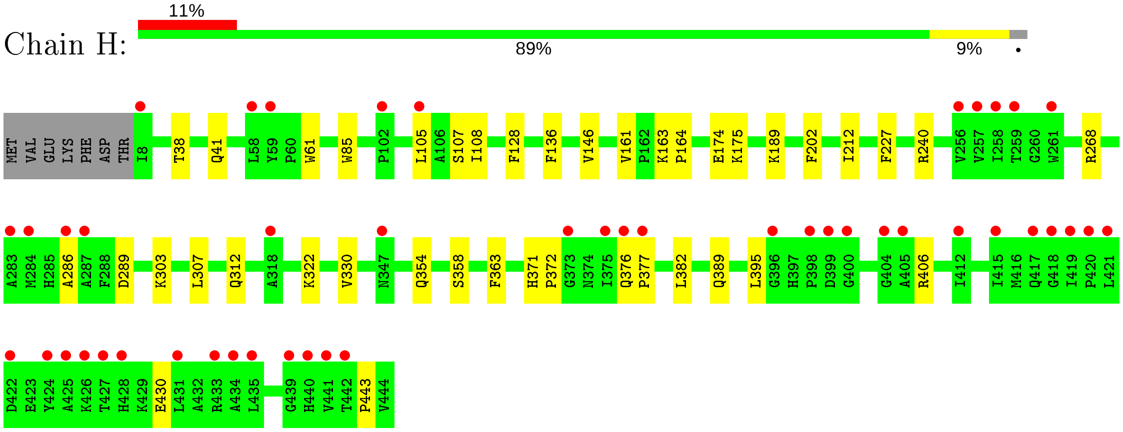
Chain G:





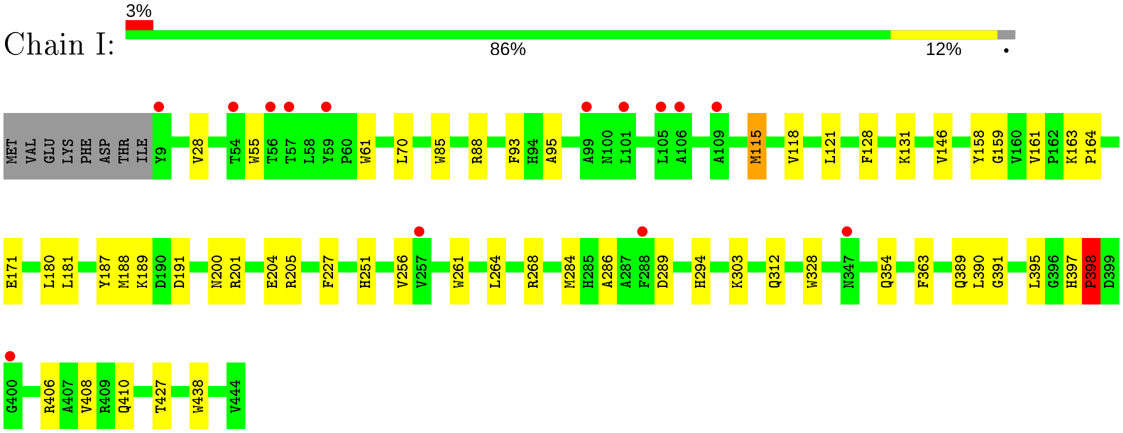
- Molecule 1: Ribulose bisphosphate carboxylase

Chain H:



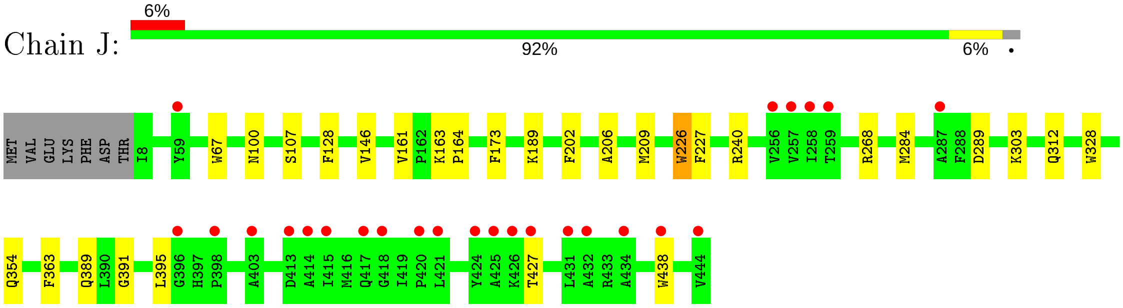
- Molecule 1: Ribulose bisphosphate carboxylase

Chain I:



- Molecule 1: Ribulose bisphosphate carboxylase

Chain J:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	170.57Å 246.24Å 144.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 47.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 99.7 (47.18-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.220 , 0.258 0.215 , 0.250	Depositor DCC
R_{free} test set	14396 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	1.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36577	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2523e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, EDO, 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	0.48	2/3502 (0.1%)	0.51	0/4753
1	B	0.48	3/3517 (0.1%)	0.50	0/4770
1	C	0.48	2/3520 (0.1%)	0.51	0/4773
1	D	0.50	5/3517 (0.1%)	0.52	0/4766
1	E	0.50	2/3515 (0.1%)	0.52	0/4767
1	F	0.49	4/3483 (0.1%)	0.51	0/4724
1	G	0.48	3/3493 (0.1%)	0.49	0/4742
1	H	0.48	2/3500 (0.1%)	0.49	0/4748
1	I	0.50	6/3510 (0.2%)	0.53	0/4757
1	J	0.50	4/3515 (0.1%)	0.52	0/4766
All	All	0.49	33/35072 (0.1%)	0.51	0/47566

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	438	TRP	CD2-CE2	5.26	1.47	1.41
1	I	438	TRP	CD2-CE2	5.19	1.47	1.41
1	F	438	TRP	CD2-CE2	5.18	1.47	1.41
1	F	226	TRP	CD2-CE2	5.18	1.47	1.41
1	C	61	TRP	CD2-CE2	5.17	1.47	1.41
1	I	261	TRP	CD2-CE2	5.17	1.47	1.41
1	A	438	TRP	CD2-CE2	5.14	1.47	1.41
1	D	328	TRP	CD2-CE2	5.12	1.47	1.41
1	E	438	TRP	CD2-CE2	5.11	1.47	1.41
1	J	438	TRP	CD2-CE2	5.08	1.47	1.41
1	I	328	TRP	CD2-CE2	5.08	1.47	1.41
1	D	261	TRP	CD2-CE2	5.08	1.47	1.41
1	F	85	TRP	CD2-CE2	5.08	1.47	1.41
1	J	226	TRP	CD2-CE2	5.08	1.47	1.41
1	D	55	TRP	CD2-CE2	5.05	1.47	1.41
1	A	226	TRP	CD2-CE2	5.05	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	TRP	CD2-CE2	5.05	1.47	1.41
1	I	61	TRP	CD2-CE2	5.04	1.47	1.41
1	F	61	TRP	CD2-CE2	5.03	1.47	1.41
1	I	85	TRP	CD2-CE2	5.03	1.47	1.41
1	H	85	TRP	CD2-CE2	5.03	1.47	1.41
1	E	328	TRP	CD2-CE2	5.03	1.47	1.41
1	H	61	TRP	CD2-CE2	5.03	1.47	1.41
1	D	61	TRP	CD2-CE2	5.01	1.47	1.41
1	G	328	TRP	CD2-CE2	5.01	1.47	1.41
1	B	261	TRP	CD2-CE2	5.01	1.47	1.41
1	I	55	TRP	CD2-CE2	5.01	1.47	1.41
1	J	67	TRP	CD2-CE2	5.01	1.47	1.41
1	G	261	TRP	CD2-CE2	5.01	1.47	1.41
1	J	328	TRP	CD2-CE2	5.01	1.47	1.41
1	B	85	TRP	CD2-CE2	5.00	1.47	1.41
1	C	85	TRP	CD2-CE2	5.00	1.47	1.41
1	G	61	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

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	3425	0	3321	16	0
1	B	3440	0	3335	25	0
1	C	3443	0	3344	17	0
1	D	3441	0	3368	22	0
1	E	3438	0	3328	17	0
1	F	3408	0	3301	31	0
1	G	3416	0	3299	18	0
1	H	3423	0	3328	21	0
1	I	3434	0	3355	35	0
1	J	3438	0	3346	12	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0	0
3	B	21	0	9	0	0
3	C	21	0	9	0	0
3	D	21	0	8	0	0
3	E	21	0	9	0	0
3	F	21	0	9	1	0
3	G	21	0	8	0	0
3	H	21	0	9	1	0
3	I	21	0	7	0	0
3	J	21	0	9	0	0
4	A	4	0	6	1	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	H	8	0	12	0	0
4	I	8	0	12	0	0
4	J	4	0	6	1	0
5	A	183	0	0	0	0
5	B	127	0	0	0	0
5	C	223	0	0	2	0
5	D	240	0	0	0	0
5	E	252	0	0	1	0
5	F	170	0	0	3	0
5	G	133	0	0	1	0
5	H	184	0	0	0	0
5	I	244	0	0	2	0
5	J	255	0	0	0	0
All	All	36577	0	33470	212	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 3.

All (212) 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:B:406:ARG:HH11	1:B:406:ARG:HG2	1.06	1.06
1:F:174:GLU:HG3	1:F:212:ILE:HD11	1.52	0.90
1:B:108:ILE:HD12	1:B:126:LEU:HD11	1.52	0.90
1:A:128:PHE:H	1:A:354:GLN:HE22	1.24	0.86
1:B:406:ARG:NH1	1:B:406:ARG:HG2	1.86	0.86
1:C:38:THR:H	1:C:41:GLN:HE21	1.30	0.80
1:C:128:PHE:H	1:C:354:GLN:HE22	1.30	0.78
1:J:128:PHE:H	1:J:354:GLN:HE22	1.32	0.76
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.68	0.75
1:B:128:PHE:H	1:B:354:GLN:HE22	1.36	0.73
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.69	0.72
1:H:128:PHE:H	1:H:354:GLN:HE22	1.39	0.71
1:B:403:ALA:HA	1:B:406:ARG:CD	2.21	0.70
1:I:115:MET:HB2	1:I:118:VAL:HG22	1.74	0.69
1:D:128:PHE:H	1:D:354:GLN:HE22	1.38	0.68
1:C:121:LEU:H	1:C:294:HIS:HD2	1.41	0.68
1:I:161:VAL:H	1:I:389:GLN:NE2	1.90	0.68
1:E:189:KCX:HG2	1:E:227:PHE:HB2	1.76	0.68
1:G:174:GLU:HG3	1:G:212:ILE:HD11	1.75	0.68
1:H:38:THR:H	1:H:41:GLN:HE21	1.42	0.67
1:G:128:PHE:H	1:G:354:GLN:HE22	1.42	0.67
1:I:128:PHE:H	1:I:354:GLN:HE22	1.40	0.67
1:D:174:GLU:HG3	1:D:212:ILE:HD11	1.77	0.66
1:E:128:PHE:H	1:E:354:GLN:HE22	1.45	0.65
1:I:161:VAL:H	1:I:389:GLN:HE21	1.46	0.64
1:I:191:ASP:HB2	5:I:658:HOH:O	1.97	0.64
1:B:403:ALA:HA	1:B:406:ARG:HD2	1.81	0.63
1:F:128:PHE:H	1:F:354:GLN:HE22	1.44	0.63
1:D:121:LEU:H	1:D:294:HIS:HD2	1.47	0.63
1:D:163:LYS:H	1:D:395:LEU:HD22	1.64	0.62
1:B:403:ALA:HA	1:B:406:ARG:HD3	1.82	0.62
1:A:161:VAL:H	1:A:389:GLN:NE2	1.98	0.61
1:I:389:GLN:C	1:I:390:LEU:HD12	2.20	0.61
1:F:78:HIS:CD2	1:F:349:VAL:HG21	2.36	0.61
1:F:121:LEU:H	1:F:294:HIS:HD2	1.49	0.60
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.83	0.60
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.84	0.60
1:H:189:KCX:HG2	1:H:227:PHE:HB2	1.84	0.60
1:G:115:MET:HB2	1:G:118:VAL:HG22	1.84	0.60
1:F:209:MET:HA	1:F:209:MET:HE2	1.84	0.59
1:I:406:ARG:O	1:I:410:GLN:HG3	2.02	0.59
1:F:222:GLU:HG3	1:F:224:LYS:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:VAL:H	1:F:389:GLN:NE2	1.99	0.59
1:C:121:LEU:H	1:C:294:HIS:CD2	2.20	0.59
1:H:406:ARG:HH11	1:H:430:GLU:HG2	1.67	0.58
1:F:337:LEU:HD22	1:F:364:PRO:HG3	1.85	0.58
1:G:189:KCX:HG2	1:G:227:PHE:HB2	1.84	0.58
1:G:65:GLU:HB2	5:G:689:HOH:O	2.04	0.58
1:C:38:THR:H	1:C:41:GLN:NE2	2.02	0.57
1:F:189:KCX:HG2	1:F:227:PHE:HB2	1.86	0.57
1:B:189:KCX:HG2	1:B:227:PHE:HB2	1.86	0.57
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.69	0.56
1:F:121:LEU:H	1:F:294:HIS:CD2	2.24	0.55
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.70	0.55
1:D:161:VAL:H	1:D:389:GLN:NE2	2.04	0.55
1:B:406:ARG:HH11	1:B:406:ARG:CG	1.97	0.55
1:A:121:LEU:H	1:A:294:HIS:HD2	1.54	0.54
1:A:189:KCX:HG2	1:A:227:PHE:HB2	1.89	0.54
1:G:161:VAL:H	1:G:389:GLN:NE2	2.06	0.54
1:A:121:LEU:H	1:A:294:HIS:CD2	2.25	0.54
1:I:121:LEU:H	1:I:294:HIS:HD2	1.55	0.54
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.72	0.53
1:B:121:LEU:H	1:B:294:HIS:HD2	1.55	0.53
1:E:410:GLN:NE2	1:E:428:HIS:HB3	2.23	0.53
1:G:163:LYS:HA	1:G:164:PRO:C	2.29	0.53
1:I:389:GLN:O	1:I:390:LEU:HD12	2.09	0.53
1:J:161:VAL:H	1:J:389:GLN:NE2	2.07	0.53
1:F:209:MET:HA	1:F:209:MET:CE	2.39	0.52
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.91	0.52
1:C:161:VAL:H	1:C:389:GLN:NE2	2.08	0.52
1:E:376:GLN:HG3	1:E:377:PRO:HD3	1.91	0.52
1:J:202:PHE:CD2	1:J:240:ARG:HG2	2.44	0.52
1:G:105:LEU:HD23	1:G:108:ILE:HD11	1.90	0.52
1:H:406:ARG:NH1	1:H:430:GLU:HG2	2.25	0.52
1:H:330:VAL:HG12	1:H:382:LEU:HD21	1.92	0.51
1:F:161:VAL:H	1:F:389:GLN:HE21	1.58	0.51
1:D:121:LEU:H	1:D:294:HIS:CD2	2.25	0.51
1:I:303:LYS:HZ3	1:I:354:GLN:HE21	1.58	0.51
1:F:286:ALA:HA	1:F:289:ASP:OD1	2.11	0.51
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.75	0.51
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.92	0.51
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.45	0.51
1:I:201:ARG:HB2	1:I:204:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:ALA:HA	1:I:289:ASP:OD1	2.10	0.51
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.09	0.51
1:C:118:VAL:HG11	1:C:121:LEU:HB2	1.93	0.51
1:I:189:KCX:HG2	1:I:227:PHE:HB2	1.94	0.50
1:D:163:LYS:HA	1:D:164:PRO:C	2.32	0.50
1:F:203:GLU:HB2	5:F:624:HOH:O	2.10	0.50
1:H:161:VAL:H	1:H:389:GLN:NE2	2.09	0.50
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.77	0.50
1:I:161:VAL:N	1:I:389:GLN:HE21	2.10	0.49
1:B:163:LYS:H	1:B:395:LEU:HD22	1.77	0.49
1:G:121:LEU:H	1:G:294:HIS:CD2	2.30	0.49
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.77	0.49
1:F:123:LEU:HG	1:F:300:VAL:HG21	1.94	0.49
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.77	0.49
1:J:189:KCX:HG2	1:J:227:PHE:HB2	1.94	0.49
1:A:200:ASN:OD1	1:A:205:ARG:HD3	2.13	0.48
1:D:230:ILE:O	1:D:237:MET:HG2	2.14	0.48
1:B:121:LEU:H	1:B:294:HIS:CD2	2.31	0.48
1:I:427:THR:HG22	5:I:827:HOH:O	2.12	0.48
1:G:121:LEU:H	1:G:294:HIS:HD2	1.60	0.48
1:B:108:ILE:CD1	1:B:126:LEU:HD11	2.35	0.48
1:E:161:VAL:H	1:E:389:GLN:NE2	2.11	0.48
1:C:189:KCX:HG2	1:C:227:PHE:HB2	1.94	0.48
1:H:358:SER:HB3	1:I:171:GLU:OE2	2.13	0.48
1:C:218:ASN:HB2	5:C:787:HOH:O	2.14	0.48
1:D:426:LYS:HG3	1:F:220:THR:O	2.13	0.48
1:F:105:LEU:HD23	1:F:108:ILE:HD11	1.96	0.48
1:J:163:LYS:HA	1:J:164:PRO:C	2.33	0.48
1:D:206:ALA:HA	1:D:226:TRP:CZ3	2.49	0.47
1:H:163:LYS:HA	1:H:164:PRO:C	2.35	0.47
1:I:256:VAL:HG12	1:I:264:LEU:HD11	1.95	0.47
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.12	0.47
1:B:78:HIS:CD2	1:B:349:VAL:HG21	2.49	0.47
1:H:286:ALA:HA	1:H:289:ASP:OD2	2.14	0.47
1:I:121:LEU:H	1:I:294:HIS:CD2	2.31	0.47
1:B:161:VAL:H	1:B:389:GLN:NE2	2.12	0.47
1:B:163:LYS:HA	1:B:164:PRO:C	2.34	0.47
1:D:48:ALA:HB1	1:D:53:GLY:HA3	1.97	0.47
1:F:366:SER:OG	1:F:378:VAL:HG11	2.15	0.47
1:I:163:LYS:HA	1:I:164:PRO:C	2.34	0.47
1:J:100:ASN:H	4:J:503:EDO:H12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:PRO:HG2	1:D:433:ARG:O	2.15	0.46
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.97	0.46
1:E:303:LYS:NZ	1:E:354:GLN:HE21	2.13	0.46
1:A:45:ALA:HB2	1:A:117:ARG:HD2	1.97	0.46
1:H:136:PHE:HB3	1:H:307:LEU:O	2.14	0.46
1:B:115:MET:HB2	1:B:118:VAL:HG12	1.98	0.46
1:D:189:KCX:HG2	1:D:227:PHE:HB2	1.98	0.46
1:G:51:SER:OG	1:G:52:THR:N	2.47	0.46
1:F:326:GLY:HA3	5:F:732:HOH:O	2.15	0.45
1:J:206:ALA:HA	1:J:226:TRP:CZ3	2.51	0.45
1:G:303:LYS:HE2	1:G:354:GLN:HG2	1.98	0.45
1:H:163:LYS:H	1:H:395:LEU:HD22	1.81	0.45
1:E:348:ASP:OD2	1:E:351:HIS:HD2	1.99	0.45
1:B:283:ALA:O	1:B:284:MET:CB	2.64	0.44
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.44
1:I:397:HIS:HA	1:I:398:PRO:HD2	1.75	0.44
1:F:427:THR:HG23	1:F:428:HIS:ND1	2.31	0.44
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.52	0.44
1:G:136:PHE:HB3	1:G:307:LEU:O	2.18	0.44
1:H:322:LYS:HA	1:H:443:PRO:O	2.17	0.44
1:C:286:ALA:HA	1:C:289:ASP:OD1	2.18	0.44
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.53	0.44
1:A:70:LEU:HD22	1:A:95:ALA:HA	2.00	0.43
1:E:163:LYS:HA	1:E:164:PRO:C	2.38	0.43
1:J:209:MET:HG2	1:J:226:TRP:CG	2.52	0.43
1:A:286:ALA:HA	1:A:289:ASP:OD2	2.18	0.43
1:B:376:GLN:N	1:B:377:PRO:HD2	2.33	0.43
1:I:70:LEU:HD22	1:I:95:ALA:HA	2.01	0.43
1:H:105:LEU:HD23	1:H:108:ILE:HD11	2.01	0.43
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.18	0.43
1:H:202:PHE:CD2	1:H:240:ARG:HG2	2.54	0.43
1:I:28:VAL:HG22	1:I:88:ARG:HG2	2.01	0.43
1:I:389:GLN:HE22	1:I:391:GLY:N	2.17	0.43
1:D:425:ALA:HB1	1:D:432:ALA:HB2	2.01	0.43
1:D:200:ASN:OD1	1:D:205:ARG:CG	2.67	0.43
1:F:220:THR:OG1	1:F:222:GLU:HG2	2.18	0.43
1:I:251:HIS:NE2	1:I:312:GLN:NE2	2.65	0.43
1:I:93:PHE:CE1	1:I:131:LYS:HE3	2.54	0.43
1:J:173:PHE:CE2	1:J:209:MET:CE	3.01	0.43
1:A:214:ASP:OD1	4:A:503:EDO:H21	2.18	0.43
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ILE:HG21	1:A:349:VAL:O	2.19	0.43
1:I:181:LEU:HD21	1:I:188:MET:HG2	2.01	0.43
1:B:203:GLU:O	1:B:207:GLU:HG2	2.18	0.42
1:H:371:HIS:HB2	1:H:372:PRO:HD2	2.01	0.42
1:H:189:KCX:CX	3:H:502:CAP:HO3	2.32	0.42
1:D:149:MET:CE	1:D:251:HIS:CE1	3.02	0.42
1:D:364:PRO:HB2	1:D:386:ILE:HG22	2.02	0.42
1:G:283:ALA:O	1:G:284:MET:CB	2.67	0.42
1:D:286:ALA:HA	1:D:289:ASP:OD1	2.19	0.42
1:D:149:MET:HE2	1:D:251:HIS:HE1	1.84	0.42
1:D:51:SER:OG	1:D:52:THR:N	2.51	0.42
1:E:139:PRO:HD3	1:E:306:ARG:O	2.19	0.42
1:A:376:GLN:HB3	1:A:377:PRO:HD3	2.01	0.42
1:E:351:HIS:HE1	5:E:709:HOH:O	2.02	0.42
1:F:163:LYS:HA	1:F:164:PRO:C	2.39	0.42
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.55	0.42
1:B:371:HIS:HB2	1:B:372:PRO:HD2	2.02	0.41
1:C:291:ASN:HA	1:C:292:PRO:HD3	1.94	0.41
1:E:70:LEU:HD22	1:E:95:ALA:HA	2.01	0.41
1:F:136:PHE:HB3	1:F:307:LEU:O	2.20	0.41
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.84	0.41
1:G:303:LYS:NZ	1:G:354:GLN:HE21	2.18	0.41
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.18	0.41
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.56	0.41
1:F:208:ILE:HG22	1:F:209:MET:HE2	2.02	0.41
1:E:93:PHE:HB2	1:E:132:LEU:HD11	2.01	0.41
1:C:117:ARG:NH2	5:C:718:HOH:O	2.53	0.41
1:C:371:HIS:HB2	1:C:372:PRO:HD2	2.03	0.41
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.85	0.41
1:F:189:KCX:CX	3:F:502:CAP:HO3	2.32	0.41
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.55	0.41
1:G:286:ALA:HA	1:G:289:ASP:OD1	2.20	0.41
1:A:63:GLU:HG2	1:A:65:GLU:HG2	2.03	0.41
1:B:286:ALA:HA	1:B:289:ASP:OD1	2.21	0.41
1:F:319:GLY:HA2	5:F:679:HOH:O	2.19	0.41
1:J:391:GLY:O	1:J:395:LEU:HD12	2.21	0.41
1:B:406:ARG:HD3	1:B:430:GLU:HG2	2.02	0.40
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.68	0.40
1:F:283:ALA:O	1:F:284:MET:CB	2.68	0.40
1:I:180:LEU:HD12	1:I:188:MET:HE1	2.03	0.40
1:E:322:LYS:HG3	1:E:323:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.52	0.40
1:D:158:TYR:CD1	1:D:408:VAL:HG11	2.57	0.40
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.21	0.40
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.85	0.40
1:H:376:GLN:HB3	1:H:377:PRO:HD3	2.03	0.40
1:I:158:TYR:CD1	1:I:408:VAL:HG11	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	415 (96%)	19 (4%)	0	100	100
1	B	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	47	55
1	C	435/444 (98%)	419 (96%)	15 (3%)	1 (0%)	47	55
1	D	433/444 (98%)	416 (96%)	16 (4%)	1 (0%)	47	55
1	E	435/444 (98%)	420 (97%)	15 (3%)	0	100	100
1	F	433/444 (98%)	417 (96%)	15 (4%)	1 (0%)	47	55
1	G	433/444 (98%)	416 (96%)	16 (4%)	1 (0%)	47	55
1	H	434/444 (98%)	417 (96%)	17 (4%)	0	100	100
1	I	433/444 (98%)	415 (96%)	16 (4%)	2 (0%)	29	29
1	J	434/444 (98%)	419 (96%)	14 (3%)	1 (0%)	47	55
All	All	4339/4440 (98%)	4168 (96%)	163 (4%)	8 (0%)	47	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	MET

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Mol	Chain	Res	Type
1	D	284	MET
1	I	284	MET
1	C	284	MET
1	G	284	MET
1	I	398	PRO
1	J	284	MET
1	F	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	339/355 (96%)	335 (99%)	4 (1%)	71	80
1	B	341/355 (96%)	336 (98%)	5 (2%)	65	75
1	C	342/355 (96%)	338 (99%)	4 (1%)	71	80
1	D	345/355 (97%)	343 (99%)	2 (1%)	86	91
1	E	340/355 (96%)	336 (99%)	4 (1%)	71	80
1	F	336/355 (95%)	331 (98%)	5 (2%)	65	75
1	G	338/355 (95%)	333 (98%)	5 (2%)	65	75
1	H	338/355 (95%)	334 (99%)	4 (1%)	71	80
1	I	343/355 (97%)	338 (98%)	5 (2%)	65	75
1	J	341/355 (96%)	336 (98%)	5 (2%)	65	75
All	All	3403/3550 (96%)	3360 (99%)	43 (1%)	69	79

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	107	SER
1	A	268	ARG
1	A	363	PHE
1	B	107	SER
1	B	268	ARG

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Mol	Chain	Res	Type
1	B	363	PHE
1	B	406	ARG
1	B	429	LYS
1	C	107	SER
1	C	268	ARG
1	C	363	PHE
1	C	429	LYS
1	D	268	ARG
1	D	363	PHE
1	E	107	SER
1	E	268	ARG
1	E	363	PHE
1	E	376	GLN
1	F	35	GLU
1	F	40	GLU
1	F	191	ASP
1	F	268	ARG
1	F	363	PHE
1	G	59	TYR
1	G	107	SER
1	G	211	LYS
1	G	268	ARG
1	G	363	PHE
1	H	107	SER
1	H	175	LYS
1	H	268	ARG
1	H	363	PHE
1	I	115	MET
1	I	268	ARG
1	I	363	PHE
1	I	395	LEU
1	I	398	PRO
1	J	107	SER
1	J	268	ARG
1	J	289	ASP
1	J	363	PHE
1	J	427	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	354	GLN
1	A	389	GLN
1	B	64	GLN
1	B	78	HIS
1	B	279	HIS
1	B	294	HIS
1	B	312	GLN
1	B	354	GLN
1	B	389	GLN
1	C	41	GLN
1	C	294	HIS
1	C	312	GLN
1	C	354	GLN
1	C	389	GLN
1	D	294	HIS
1	D	312	GLN
1	D	354	GLN
1	D	389	GLN
1	E	312	GLN
1	E	351	HIS
1	E	354	GLN
1	E	389	GLN
1	E	410	GLN
1	F	78	HIS
1	F	294	HIS
1	F	312	GLN
1	F	354	GLN
1	F	389	GLN
1	G	279	HIS
1	G	294	HIS
1	G	312	GLN
1	G	354	GLN
1	G	389	GLN
1	H	41	GLN
1	H	279	HIS
1	H	294	HIS
1	H	312	GLN
1	H	354	GLN
1	H	389	GLN
1	I	294	HIS
1	I	312	GLN

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Mol	Chain	Res	Type
1	I	332	GLN
1	I	354	GLN
1	I	389	GLN
1	J	312	GLN
1	J	354	GLN
1	J	389	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	G	189	1,2	7,11,12	0.42	0	4,12,14	0.58	0
1	KCX	C	189	1,2	7,11,12	0.46	0	4,12,14	0.38	0
1	KCX	I	189	1,2	7,11,12	0.50	0	4,12,14	0.44	0
1	KCX	F	189	1,2	7,11,12	0.51	0	4,12,14	0.57	0
1	KCX	D	189	1,2	7,11,12	0.51	0	4,12,14	0.36	0
1	KCX	B	189	1,2	7,11,12	0.45	0	4,12,14	0.48	0
1	KCX	J	189	1,2	7,11,12	0.45	0	4,12,14	0.47	0
1	KCX	E	189	1,2	7,11,12	0.46	0	4,12,14	0.47	0
1	KCX	H	189	1,2	7,11,12	0.44	0	4,12,14	0.49	0
1	KCX	A	189	1,2	7,11,12	0.46	0	4,12,14	0.66	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	G	189	1,2	-	0/7/10/12	-
1	KCX	C	189	1,2	-	0/7/10/12	-
1	KCX	I	189	1,2	-	0/7/10/12	-
1	KCX	F	189	1,2	-	0/7/10/12	-
1	KCX	D	189	1,2	-	0/7/10/12	-
1	KCX	B	189	1,2	-	0/7/10/12	-
1	KCX	J	189	1,2	-	0/7/10/12	-
1	KCX	E	189	1,2	-	0/7/10/12	-
1	KCX	H	189	1,2	-	0/7/10/12	-
1	KCX	A	189	1,2	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	C	189	KCX	1	0
1	I	189	KCX	1	0
1	F	189	KCX	2	0
1	D	189	KCX	1	0
1	B	189	KCX	1	0
1	J	189	KCX	1	0
1	E	189	KCX	1	0
1	H	189	KCX	2	0
1	A	189	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	B	502	2	15,20,20	0.62	0	20,31,31	0.99	0
4	EDO	E	503	-	3,3,3	0.55	0	2,2,2	0.14	0
3	CAP	G	502	2	15,20,20	0.61	0	20,31,31	1.02	0
3	CAP	D	502	2	15,20,20	0.66	0	20,31,31	0.99	0
3	CAP	E	502	2	15,20,20	0.67	0	20,31,31	0.92	0
4	EDO	I	503	-	3,3,3	0.50	0	2,2,2	0.20	0
3	CAP	C	502	2	15,20,20	0.58	0	20,31,31	1.00	0
4	EDO	A	503	-	3,3,3	0.52	0	2,2,2	0.13	0
3	CAP	A	502	2	15,20,20	0.58	0	20,31,31	1.04	0
3	CAP	F	502	2	15,20,20	0.60	0	20,31,31	1.05	1 (5%)
4	EDO	H	504	-	3,3,3	0.52	0	2,2,2	0.20	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	D	503	-	3,3,3	0.44	0	2,2,2	0.41	0
3	CAP	H	502	2	15,20,20	0.58	0	20,31,31	0.96	0
3	CAP	I	502	2	15,20,20	0.62	0	20,31,31	1.09	1 (5%)
4	EDO	H	503	-	3,3,3	0.47	0	2,2,2	0.27	0
3	CAP	J	502	2	15,20,20	0.66	0	20,31,31	0.93	0
4	EDO	J	503	-	3,3,3	0.68	0	2,2,2	0.16	0
4	EDO	I	504	-	3,3,3	0.54	0	2,2,2	0.14	0
4	EDO	C	503	-	3,3,3	0.50	0	2,2,2	0.24	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
3	CAP	B	502	2	-	3/23/29/29	-
4	EDO	E	503	-	-	1/1/1/1	-
3	CAP	G	502	2	-	2/23/29/29	-
3	CAP	D	502	2	-	2/23/29/29	-
3	CAP	E	502	2	-	7/23/29/29	-
4	EDO	I	503	-	-	0/1/1/1	-
3	CAP	C	502	2	-	3/23/29/29	-
4	EDO	A	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	A	502	2	-	4/23/29/29	-
3	CAP	F	502	2	-	3/23/29/29	-
4	EDO	H	504	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
3	CAP	H	502	2	-	4/23/29/29	-
3	CAP	I	502	2	-	2/23/29/29	-
4	EDO	H	503	-	-	0/1/1/1	-
3	CAP	J	502	2	-	5/23/29/29	-
4	EDO	J	503	-	-	0/1/1/1	-
4	EDO	I	504	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	502	CAP	O6P-P2-O5P	2.40	116.81	107.64
3	I	502	CAP	O6P-P2-O5P	2.11	115.69	107.64

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	CAP	O3-C3-C4-O4
3	D	502	CAP	O3-C3-C4-O4
3	E	502	CAP	C2-C3-C4-O4
3	E	502	CAP	O3-C3-C4-O4
3	F	502	CAP	C2-C3-C4-O4
3	F	502	CAP	O3-C3-C4-O4
3	I	502	CAP	O3-C3-C4-O4
3	J	502	CAP	O3-C3-C4-O4
3	C	502	CAP	O3-C3-C4-O4
3	A	502	CAP	O3-C3-C4-O4
3	H	502	CAP	O3-C3-C4-O4
3	B	502	CAP	O2-C2-C3-C4
3	D	502	CAP	O2-C2-C3-C4
3	E	502	CAP	O2-C2-C3-C4
3	F	502	CAP	O2-C2-C3-C4
3	I	502	CAP	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	J	502	CAP	O2-C2-C3-C4
3	C	502	CAP	O2-C2-C3-C4
3	A	502	CAP	O2-C2-C3-C4
3	H	502	CAP	O2-C2-C3-C4
3	G	502	CAP	O2-C2-C3-C4
3	A	502	CAP	C2-C3-C4-O4
3	G	502	CAP	O3-C3-C4-O4
3	J	502	CAP	O1-C1-C2-O2
3	J	502	CAP	C2-C3-C4-O4
3	H	502	CAP	C2-C3-C4-O4
3	H	502	CAP	C5-O5-P2-O4P
4	H	504	EDO	O1-C1-C2-O2
3	E	502	CAP	C4-C5-O5-P2
3	E	502	CAP	O4-C4-C5-O5
3	J	502	CAP	O4-C4-C5-O5
3	C	502	CAP	O4-C4-C5-O5
3	A	502	CAP	O4-C4-C5-O5
3	E	502	CAP	C5-O5-P2-O4P
4	E	503	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
3	E	502	CAP	C2-C3-C4-C5
3	B	502	CAP	O4-C4-C5-O5

There are no ring outliers.

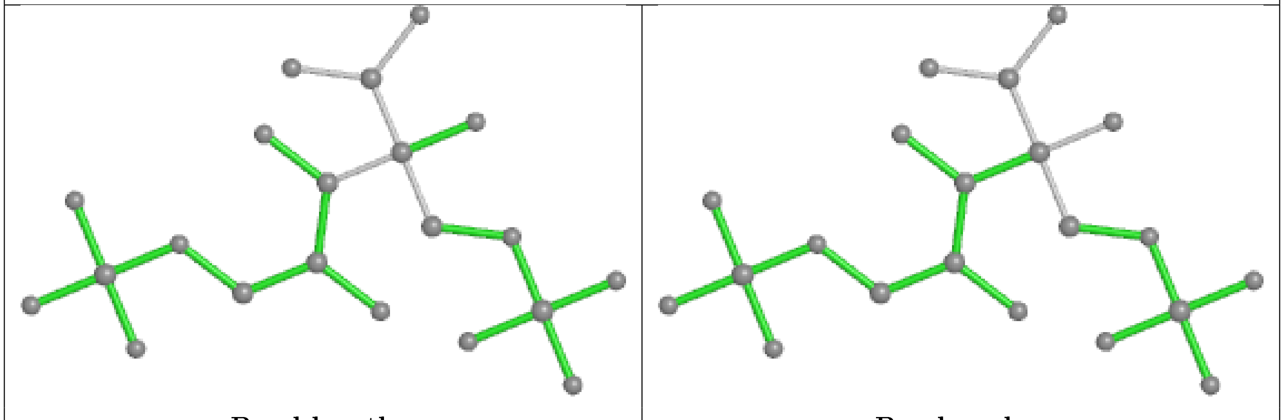
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	EDO	1	0
3	F	502	CAP	1	0
3	H	502	CAP	1	0
4	J	503	EDO	1	0

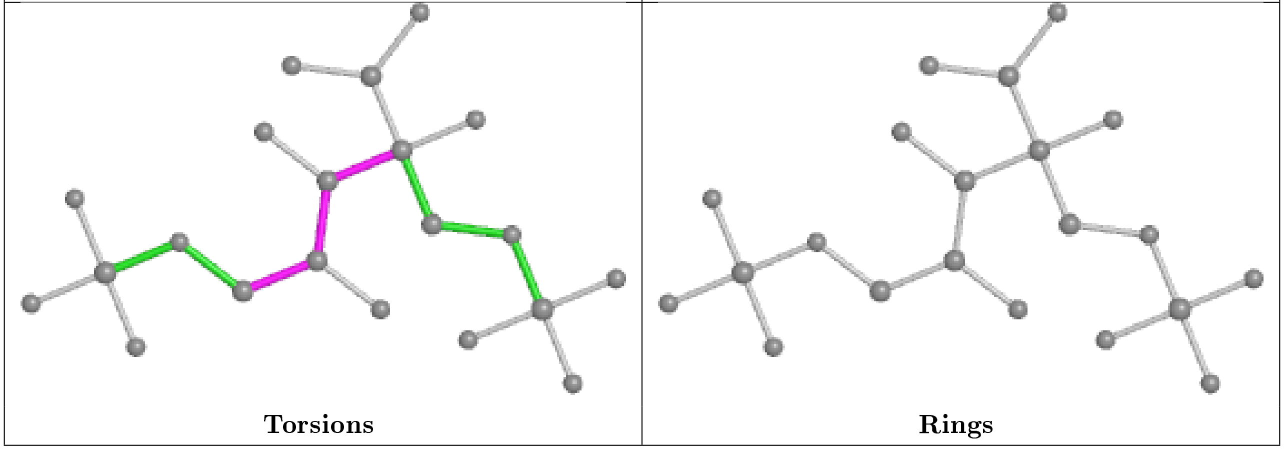
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CAP B 502

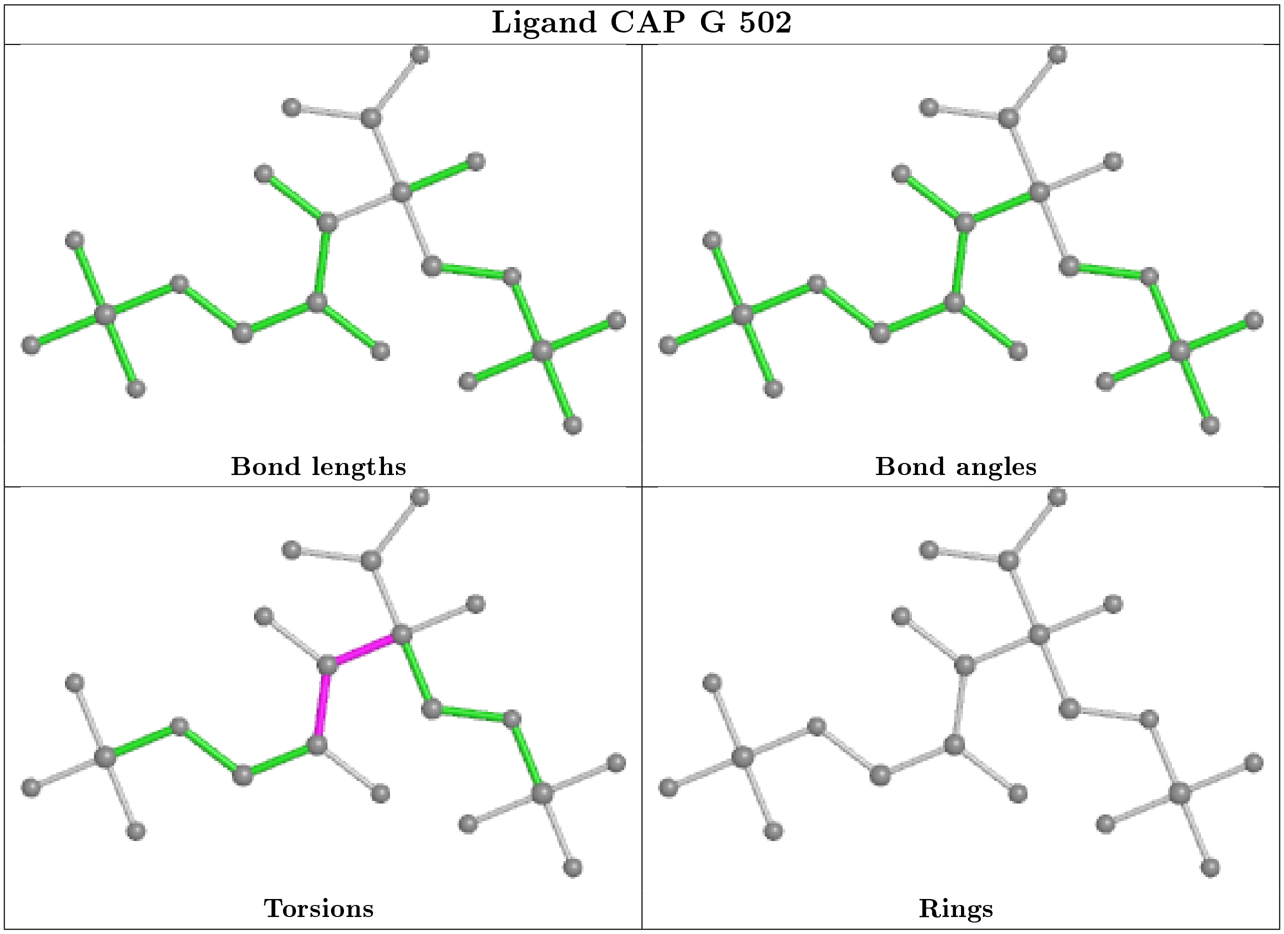


Bond lengths Bond angles



Torsions Rings

Ligand CAP G 502



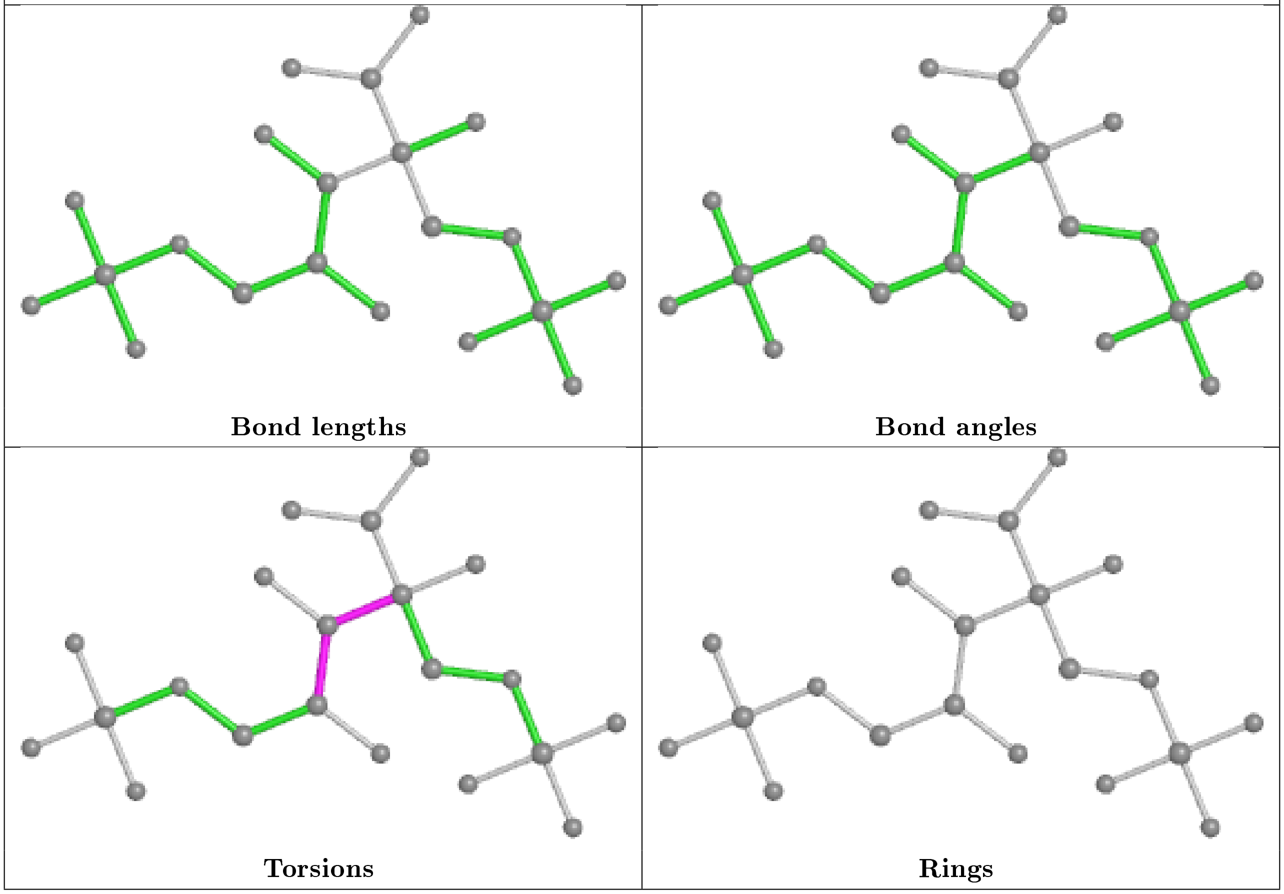
Bond lengths

Bond angles

Torsions

Rings

Ligand CAP D 502



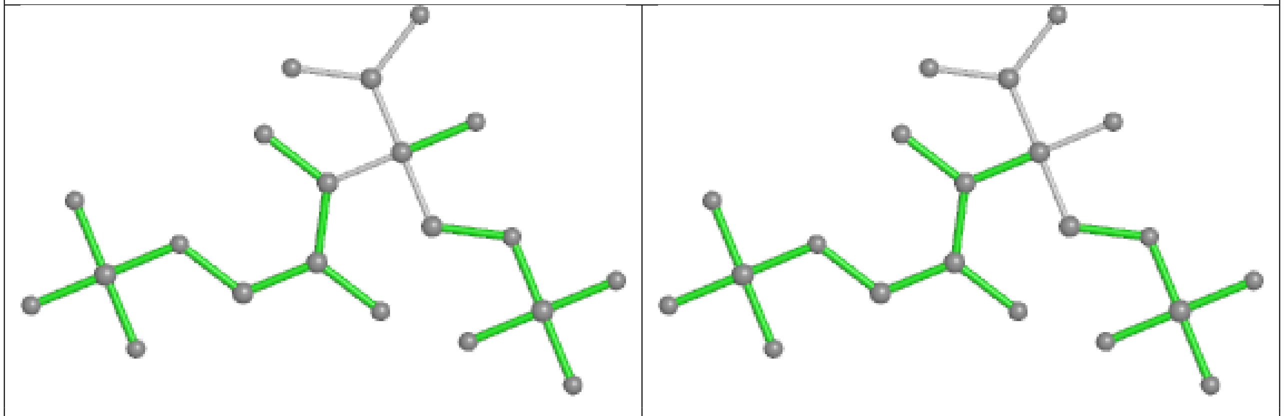
Bond lengths

Bond angles

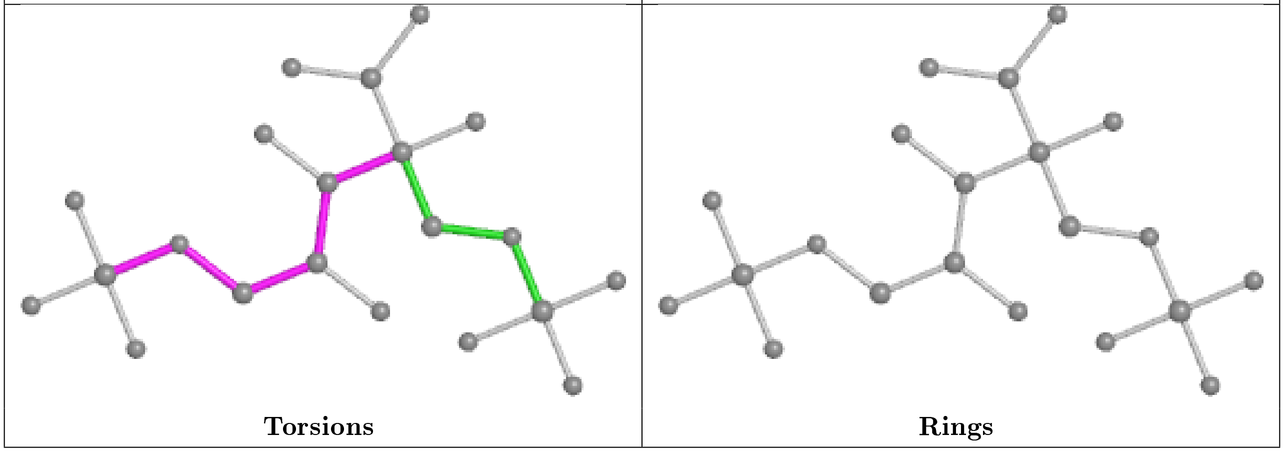
Torsions

Rings

Ligand CAP E 502

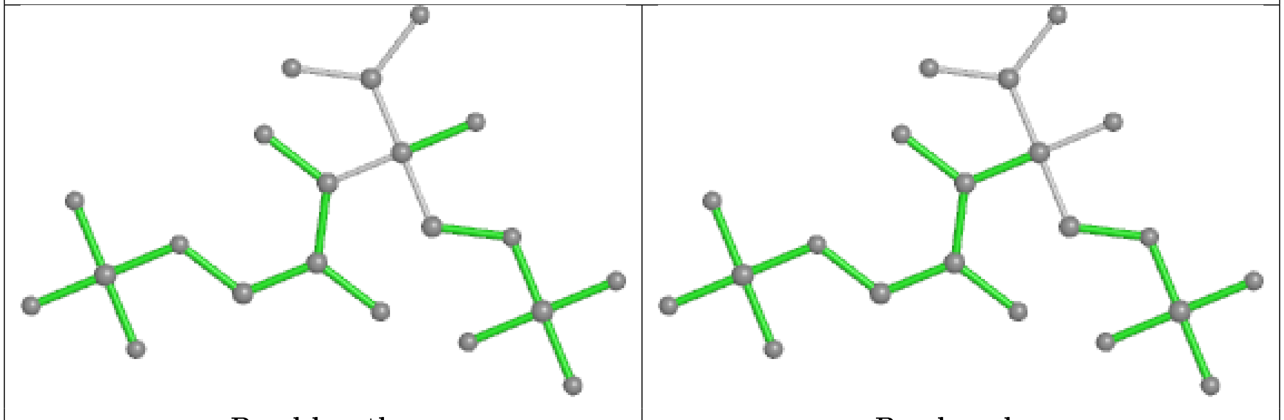


Bond lengths **Bond angles**

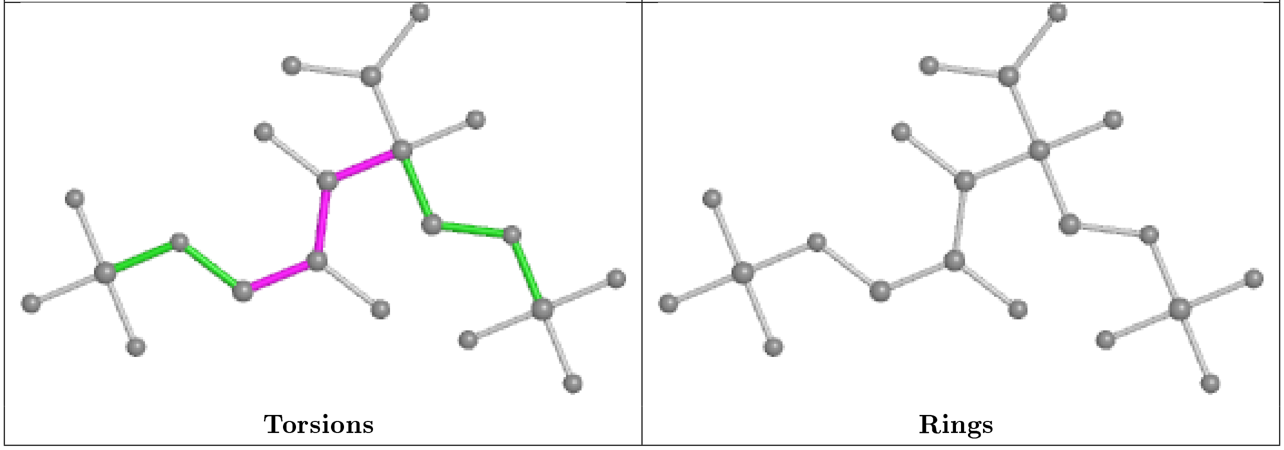


Torsions **Rings**

Ligand CAP C 502

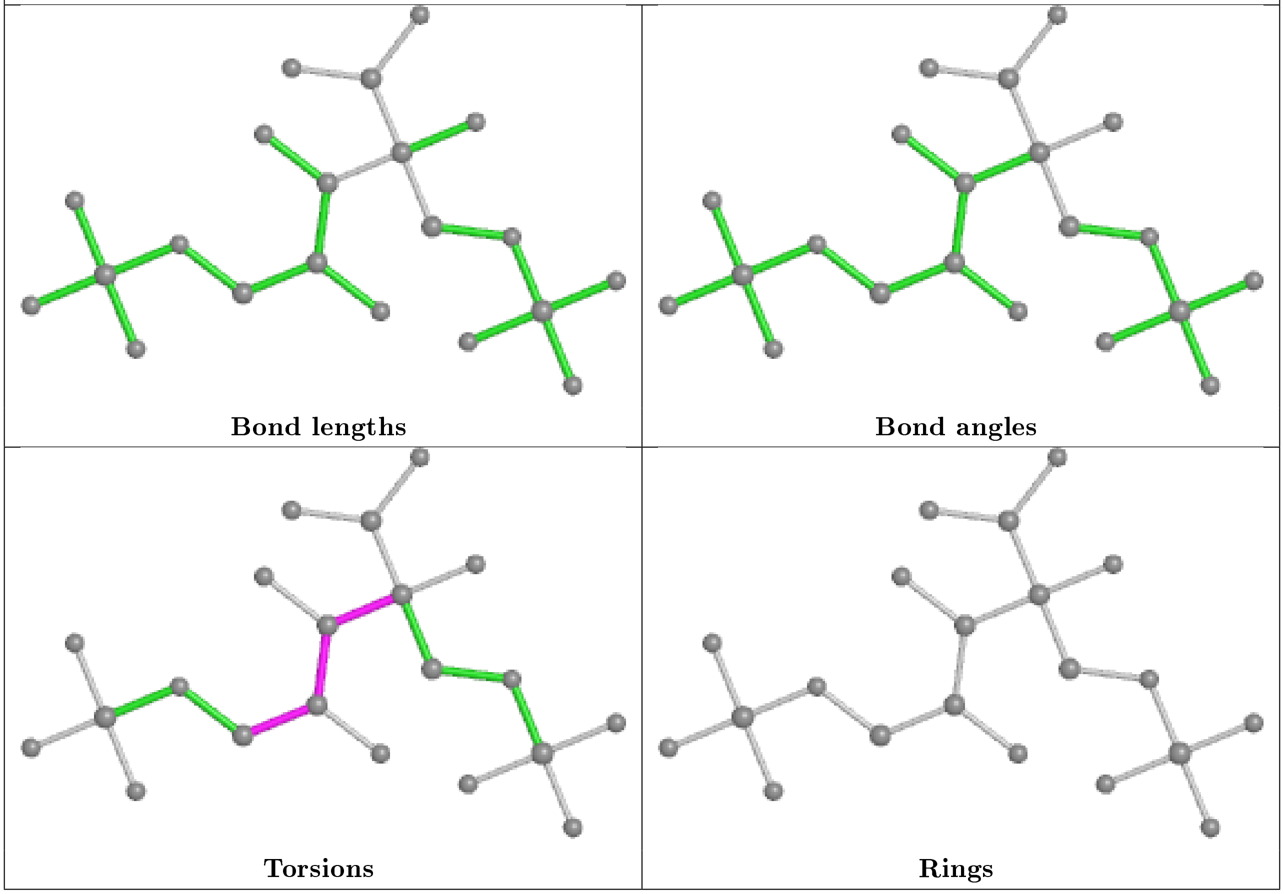


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CAP A 502



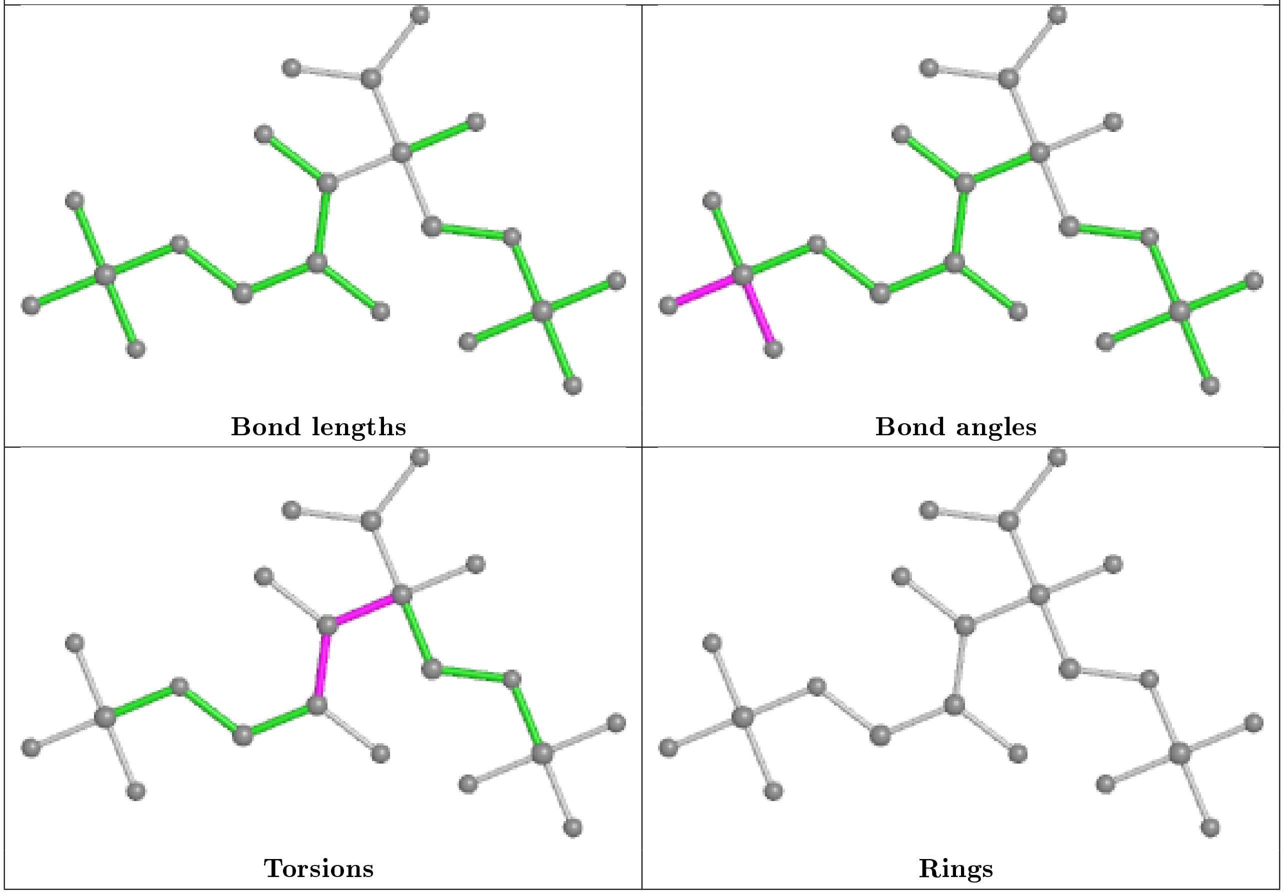
Bond lengths

Bond angles

Torsions

Rings

Ligand CAP F 502



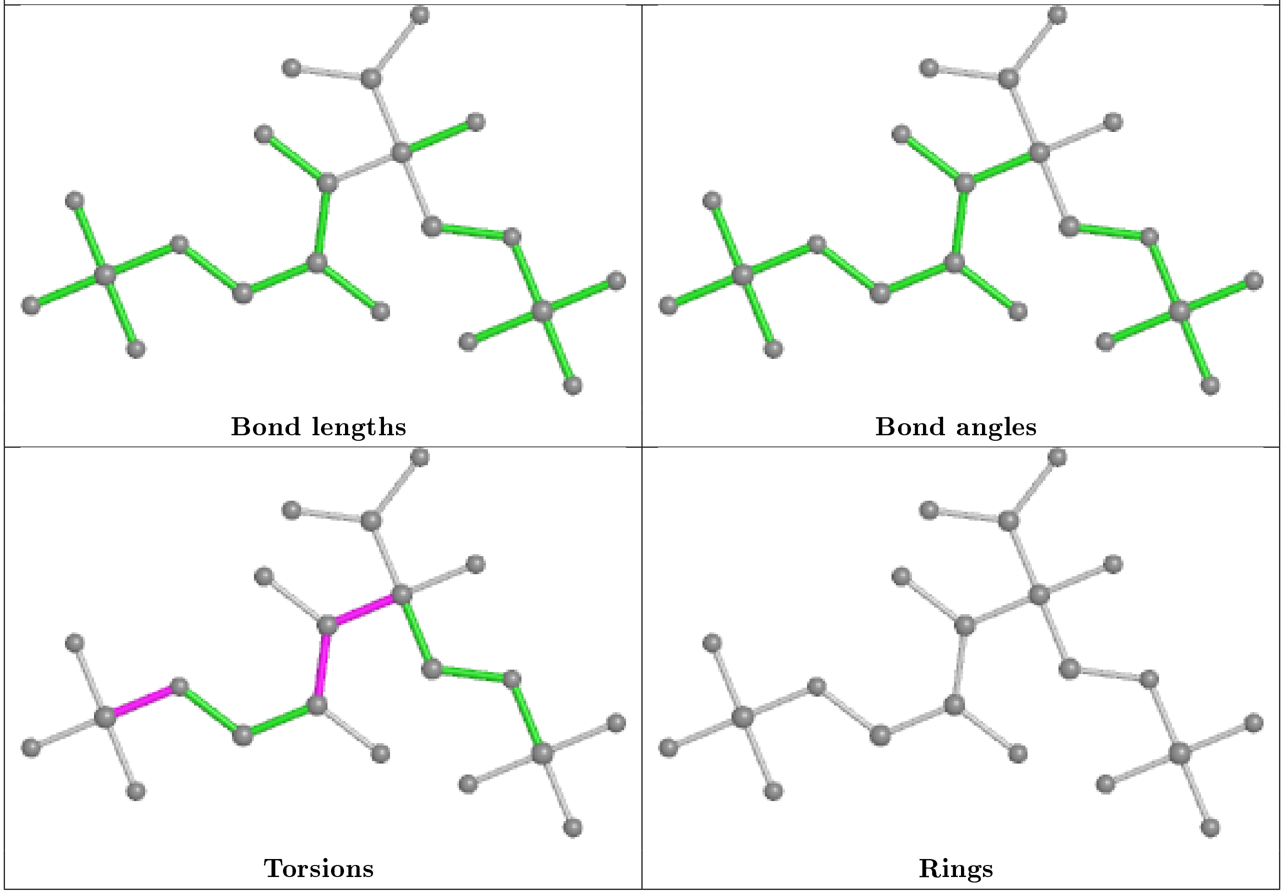
Bond lengths

Bond angles

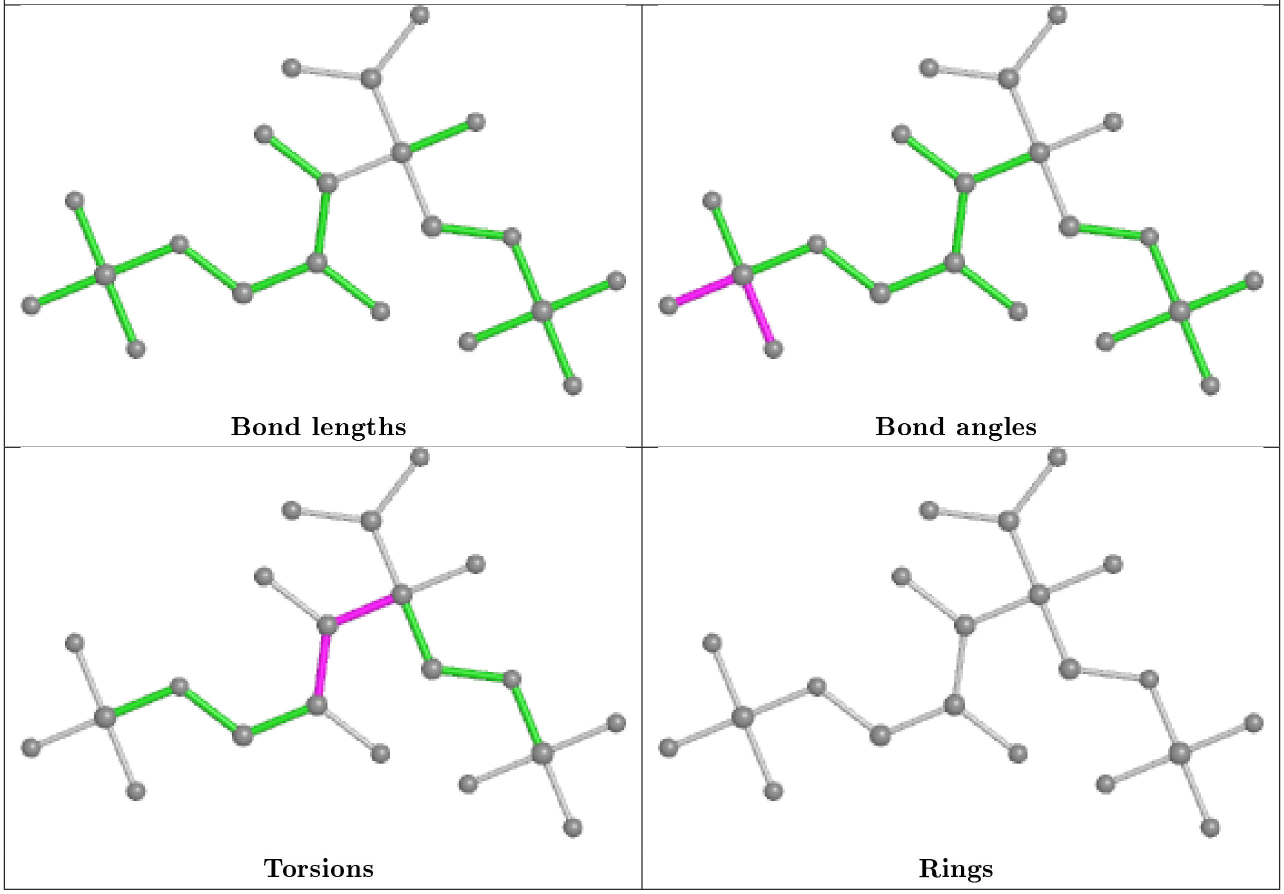
Torsions

Rings

Ligand CAP H 502



Ligand CAP I 502



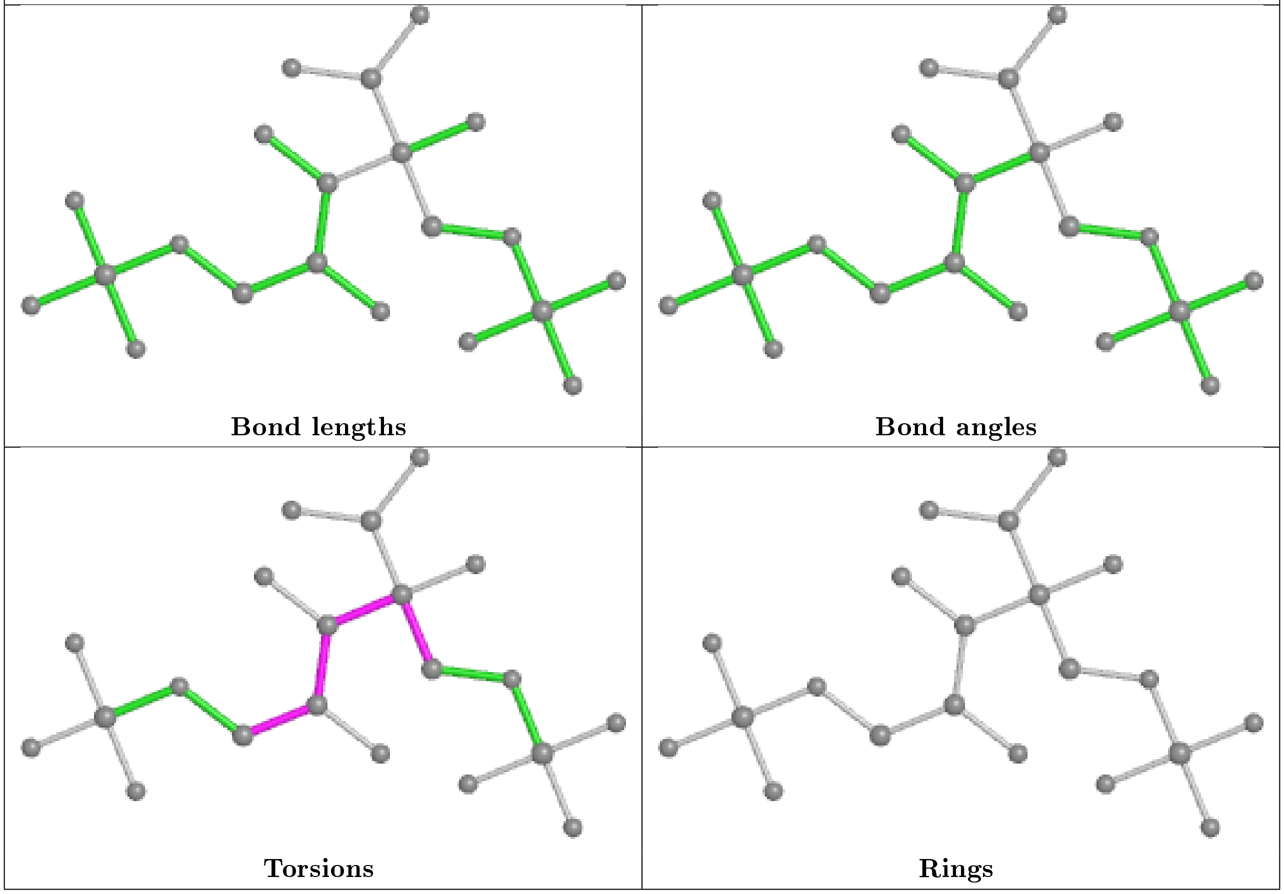
Bond lengths

Bond angles

Torsions

Rings

Ligand CAP J 502



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	436/444 (98%)	0.17	20 (4%)	32	35	30, 49, 71, 89	0
1	B	437/444 (98%)	0.48	43 (9%)	7	8	38, 58, 90, 108	0
1	C	437/444 (98%)	0.07	20 (4%)	32	35	28, 43, 76, 95	0
1	D	435/444 (97%)	0.29	31 (7%)	16	17	26, 50, 80, 93	0
1	E	437/444 (98%)	0.13	29 (6%)	18	20	24, 42, 84, 101	0
1	F	435/444 (97%)	0.53	40 (9%)	9	9	32, 62, 94, 123	0
1	G	435/444 (97%)	0.64	62 (14%)	2	2	40, 58, 87, 109	0
1	H	436/444 (98%)	0.39	47 (10%)	5	5	32, 53, 95, 122	0
1	I	435/444 (97%)	0.08	14 (3%)	47	50	25, 46, 77, 92	0
1	J	436/444 (98%)	0.08	25 (5%)	23	25	25, 40, 79, 96	0
All	All	4359/4440 (98%)	0.29	331 (7%)	13	15	24, 50, 85, 123	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	421	LEU	6.0
1	A	59	TYR	5.6
1	J	414	ALA	5.5
1	I	9	TYR	5.3
1	G	421	LEU	5.3
1	D	9	TYR	5.3
1	J	444	VAL	5.1
1	F	414	ALA	4.8
1	G	258	ILE	4.8
1	G	257	VAL	4.8
1	A	8	ILE	4.7
1	G	414	ALA	4.6
1	G	410	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	58	LEU	4.6
1	H	424	TYR	4.5
1	H	434	ALA	4.5
1	D	54	THR	4.5
1	C	421	LEU	4.4
1	G	403	ALA	4.4
1	J	424	TYR	4.4
1	G	284	MET	4.4
1	G	287	ALA	4.4
1	G	283	ALA	4.4
1	G	16	GLY	4.3
1	G	59	TYR	4.3
1	F	421	LEU	4.3
1	H	441	VAL	4.3
1	H	427	THR	4.3
1	G	256	VAL	4.2
1	B	398	PRO	4.2
1	B	288	PHE	4.2
1	A	257	VAL	4.1
1	F	16	GLY	4.1
1	B	8	ILE	4.0
1	H	396	GLY	4.0
1	H	417	GLN	4.0
1	B	57	THR	4.0
1	G	296	ILE	3.9
1	D	261	TRP	3.9
1	B	287	ALA	3.9
1	B	414	ALA	3.9
1	G	109	ALA	3.9
1	G	288	PHE	3.9
1	H	439	GLY	3.9
1	J	417	GLN	3.9
1	E	258	ILE	3.8
1	H	419	ILE	3.8
1	G	261	TRP	3.8
1	B	296	ILE	3.7
1	G	105	LEU	3.7
1	F	424	TYR	3.7
1	G	426	LYS	3.7
1	F	441	VAL	3.7
1	F	398	PRO	3.7
1	I	347	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	284	MET	3.6
1	C	419	ILE	3.6
1	D	58	LEU	3.6
1	E	444	VAL	3.6
1	G	424	TYR	3.6
1	G	346	GLU	3.6
1	J	425	ALA	3.5
1	D	257	VAL	3.5
1	B	258	ILE	3.5
1	D	105	LEU	3.5
1	G	106	ALA	3.5
1	D	347	ASN	3.5
1	B	152	ILE	3.5
1	B	283	ALA	3.5
1	E	434	ALA	3.4
1	C	420	PRO	3.4
1	B	439	GLY	3.4
1	J	418	GLY	3.4
1	D	59	TYR	3.4
1	F	256	VAL	3.3
1	H	283	ALA	3.3
1	F	376	GLN	3.3
1	D	101	LEU	3.3
1	D	56	THR	3.3
1	C	59	TYR	3.3
1	H	59	TYR	3.2
1	H	257	VAL	3.2
1	B	434	ALA	3.2
1	B	105	LEU	3.2
1	G	101	LEU	3.2
1	B	85	TRP	3.2
1	J	59	TYR	3.2
1	C	441	VAL	3.2
1	B	417	GLN	3.1
1	H	376	GLN	3.1
1	H	400	GLY	3.1
1	H	412	ILE	3.1
1	G	113	PHE	3.1
1	F	425	ALA	3.1
1	A	418	GLY	3.1
1	G	11	TYR	3.1
1	C	258	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	373	GLY	3.1
1	F	403	ALA	3.1
1	F	417	GLN	3.1
1	F	257	VAL	3.0
1	B	59	TYR	3.0
1	J	431	LEU	3.0
1	D	346	GLU	3.0
1	H	431	LEU	3.0
1	I	59	TYR	3.0
1	H	418	GLY	3.0
1	G	57	THR	3.0
1	H	420	PRO	3.0
1	C	426	LYS	3.0
1	D	258	ILE	3.0
1	F	432	ALA	3.0
1	D	256	VAL	3.0
1	E	256	VAL	3.0
1	E	257	VAL	3.0
1	B	400	GLY	2.9
1	B	256	VAL	2.9
1	B	257	VAL	2.9
1	G	347	ASN	2.9
1	I	54	THR	2.9
1	J	421	LEU	2.9
1	B	396	GLY	2.9
1	A	256	VAL	2.9
1	G	259	THR	2.9
1	B	410	GLN	2.9
1	E	421	LEU	2.9
1	A	258	ILE	2.9
1	I	57	THR	2.9
1	B	113	PHE	2.9
1	G	285	HIS	2.9
1	H	258	ILE	2.8
1	F	420	PRO	2.8
1	A	9	TYR	2.8
1	D	288	PHE	2.8
1	A	101	LEU	2.8
1	D	102	PRO	2.8
1	E	400	GLY	2.8
1	C	257	VAL	2.8
1	D	109	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	403	ALA	2.8
1	H	442	THR	2.8
1	E	376	GLN	2.8
1	C	376	GLN	2.7
1	H	375	ILE	2.7
1	C	398	PRO	2.7
1	G	398	PRO	2.7
1	B	261	TRP	2.7
1	G	418	GLY	2.7
1	G	152	ILE	2.7
1	J	398	PRO	2.7
1	D	55	TRP	2.7
1	G	222	GLU	2.7
1	G	54	THR	2.7
1	H	399	ASP	2.7
1	D	283	ALA	2.7
1	G	431	LEU	2.7
1	H	398	PRO	2.7
1	B	403	ALA	2.7
1	H	284	MET	2.7
1	G	17	TYR	2.7
1	E	7	THR	2.7
1	B	404	GLY	2.7
1	G	60	PRO	2.6
1	D	259	THR	2.6
1	A	380	GLU	2.6
1	F	416	MET	2.6
1	G	9	TYR	2.6
1	G	412	ILE	2.6
1	F	57	THR	2.6
1	B	301	LEU	2.6
1	A	347	ASN	2.6
1	E	442	THR	2.6
1	G	264	LEU	2.6
1	I	105	LEU	2.6
1	H	404	GLY	2.6
1	F	101	LEU	2.5
1	G	104	LEU	2.5
1	G	10	ASP	2.5
1	F	106	ALA	2.5
1	H	347	ASN	2.5
1	D	57	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	435	LEU	2.5
1	G	416	MET	2.5
1	G	305	TYR	2.5
1	A	109	ALA	2.5
1	C	427	THR	2.5
1	G	102	PRO	2.5
1	B	223	LYS	2.5
1	C	373	GLY	2.5
1	G	301	LEU	2.5
1	J	257	VAL	2.5
1	J	432	ALA	2.5
1	B	401	PRO	2.5
1	H	415	ILE	2.5
1	B	436	GLU	2.5
1	F	405	ALA	2.5
1	G	419	ILE	2.5
1	D	260	GLY	2.5
1	F	423	GLU	2.5
1	D	85	TRP	2.5
1	E	380	GLU	2.5
1	F	412	ILE	2.5
1	F	58	LEU	2.5
1	F	399	ASP	2.5
1	F	435	LEU	2.5
1	A	57	THR	2.4
1	B	285	HIS	2.4
1	F	36	GLY	2.4
1	I	257	VAL	2.4
1	C	418	GLY	2.4
1	F	59	TYR	2.4
1	F	18	GLU	2.4
1	F	258	ILE	2.4
1	H	105	LEU	2.4
1	E	284	MET	2.4
1	F	347	ASN	2.4
1	G	405	ALA	2.4
1	H	428	HIS	2.4
1	F	427	THR	2.4
1	B	412	ILE	2.4
1	J	434	ALA	2.4
1	C	422	ASP	2.4
1	J	426	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	11	TYR	2.4
1	C	417	GLN	2.4
1	F	261	TRP	2.4
1	J	438	TRP	2.4
1	E	433	ARG	2.4
1	C	284	MET	2.4
1	J	427	THR	2.4
1	J	258	ILE	2.4
1	A	260	GLY	2.4
1	B	260	GLY	2.4
1	A	421	LEU	2.4
1	F	43	ALA	2.4
1	H	102	PRO	2.4
1	A	259	THR	2.4
1	A	254	VAL	2.4
1	G	18	GLU	2.4
1	J	256	VAL	2.4
1	A	16	GLY	2.3
1	H	318	ALA	2.3
1	G	375	ILE	2.3
1	B	109	ALA	2.3
1	B	421	LEU	2.3
1	G	153	LYS	2.3
1	H	256	VAL	2.3
1	H	440	HIS	2.3
1	H	377	PRO	2.3
1	E	425	ALA	2.3
1	G	81	GLY	2.3
1	G	103	GLY	2.3
1	H	426	LYS	2.3
1	G	392	GLY	2.3
1	F	440	HIS	2.2
1	G	218	ASN	2.2
1	F	109	ALA	2.2
1	F	419	ILE	2.2
1	E	231	THR	2.2
1	E	287	ALA	2.2
1	E	439	GLY	2.2
1	I	106	ALA	2.2
1	J	259	THR	2.2
1	J	413	ASP	2.2
1	F	284	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	424	TYR	2.2
1	B	433	ARG	2.2
1	C	256	VAL	2.2
1	E	105	LEU	2.2
1	E	395	LEU	2.2
1	I	101	LEU	2.2
1	D	284	MET	2.2
1	J	420	PRO	2.2
1	G	260	GLY	2.2
1	D	285	HIS	2.2
1	H	259	THR	2.2
1	I	56	THR	2.2
1	D	108	ILE	2.2
1	H	8	ILE	2.2
1	D	305	TYR	2.2
1	B	184	GLY	2.2
1	E	414	ALA	2.2
1	F	318	ALA	2.2
1	H	261	TRP	2.2
1	B	380	GLU	2.2
1	F	433	ARG	2.1
1	D	99	ALA	2.1
1	G	295	GLY	2.1
1	J	396	GLY	2.1
1	E	418	GLY	2.1
1	E	261	TRP	2.1
1	H	286	ALA	2.1
1	H	405	ALA	2.1
1	I	109	ALA	2.1
1	F	422	ASP	2.1
1	C	346	GLU	2.1
1	C	439	GLY	2.1
1	F	296	ILE	2.1
1	G	223	LYS	2.1
1	G	413	ASP	2.1
1	B	286	ALA	2.1
1	B	407	ALA	2.1
1	G	151	GLU	2.1
1	H	433	ARG	2.1
1	E	396	GLY	2.1
1	J	415	ILE	2.1
1	D	104	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	430	GLU	2.1
1	E	259	THR	2.1
1	B	150	LEU	2.1
1	H	58	LEU	2.1
1	I	400	GLY	2.1
1	B	17	TYR	2.1
1	H	422	ASP	2.0
1	D	264	LEU	2.0
1	A	218	ASN	2.0
1	E	106	ALA	2.0
1	H	287	ALA	2.0
1	H	425	ALA	2.0
1	J	287	ALA	2.0
1	G	297	SER	2.0
1	E	441	VAL	2.0
1	I	288	PHE	2.0
1	A	110	GLY	2.0
1	G	286	ALA	2.0
1	E	397	HIS	2.0
1	E	438	TRP	2.0
1	A	422	ASP	2.0
1	D	286	ALA	2.0
1	E	109	ALA	2.0
1	I	99	ALA	2.0

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

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	F	189	12/13	0.95	0.18	42,43,44,46	0
1	KCX	I	189	12/13	0.96	0.15	26,27,28,29	0
1	KCX	J	189	12/13	0.96	0.10	37,38,39,39	0
1	KCX	B	189	12/13	0.97	0.12	48,49,50,51	0
1	KCX	G	189	12/13	0.97	0.12	48,49,50,51	0
1	KCX	E	189	12/13	0.97	0.12	38,40,41,41	0
1	KCX	H	189	12/13	0.97	0.10	48,49,51,52	0
1	KCX	C	189	12/13	0.98	0.11	39,41,42,42	0
1	KCX	D	189	12/13	0.98	0.15	30,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	KCX	A	189	12/13	0.98	0.14	34,35,36,36	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
4	EDO	J	503	4/4	0.58	0.27	32,32,33,33	0
4	EDO	A	503	4/4	0.71	0.14	62,62,63,64	0
4	EDO	E	503	4/4	0.76	0.18	42,43,44,44	0
4	EDO	I	504	4/4	0.79	0.17	48,48,49,50	0
4	EDO	H	504	4/4	0.88	0.18	50,53,53,54	0
2	MG	B	501	1/1	0.88	0.14	59,59,59,59	0
2	MG	J	501	1/1	0.90	0.16	43,43,43,43	0
2	MG	E	501	1/1	0.92	0.16	45,45,45,45	0
2	MG	H	501	1/1	0.93	0.18	58,58,58,58	0
3	CAP	J	502	21/21	0.94	0.15	41,47,53,54	0
4	EDO	I	503	4/4	0.95	0.15	26,26,26,28	0
3	CAP	B	502	21/21	0.95	0.14	55,59,65,66	0
3	CAP	G	502	21/21	0.95	0.15	52,56,62,62	0
3	CAP	E	502	21/21	0.95	0.14	45,50,57,58	0
2	MG	C	501	1/1	0.95	0.10	46,46,46,46	0
3	CAP	H	502	21/21	0.95	0.13	56,60,67,68	0
3	CAP	F	502	21/21	0.96	0.14	49,53,56,57	0
2	MG	I	501	1/1	0.96	0.12	28,28,28,28	0
4	EDO	D	503	4/4	0.96	0.14	28,28,29,30	0
2	MG	F	501	1/1	0.96	0.13	46,46,46,46	0
2	MG	A	501	1/1	0.96	0.13	36,36,36,36	0
3	CAP	I	502	21/21	0.97	0.14	31,33,35,36	0
3	CAP	C	502	21/21	0.97	0.12	43,47,51,52	0
3	CAP	A	502	21/21	0.97	0.12	37,39,42,43	0
4	EDO	H	503	4/4	0.97	0.17	29,29,30,32	0
4	EDO	C	503	4/4	0.97	0.14	24,25,25,26	0
2	MG	G	501	1/1	0.97	0.15	57,57,57,57	0

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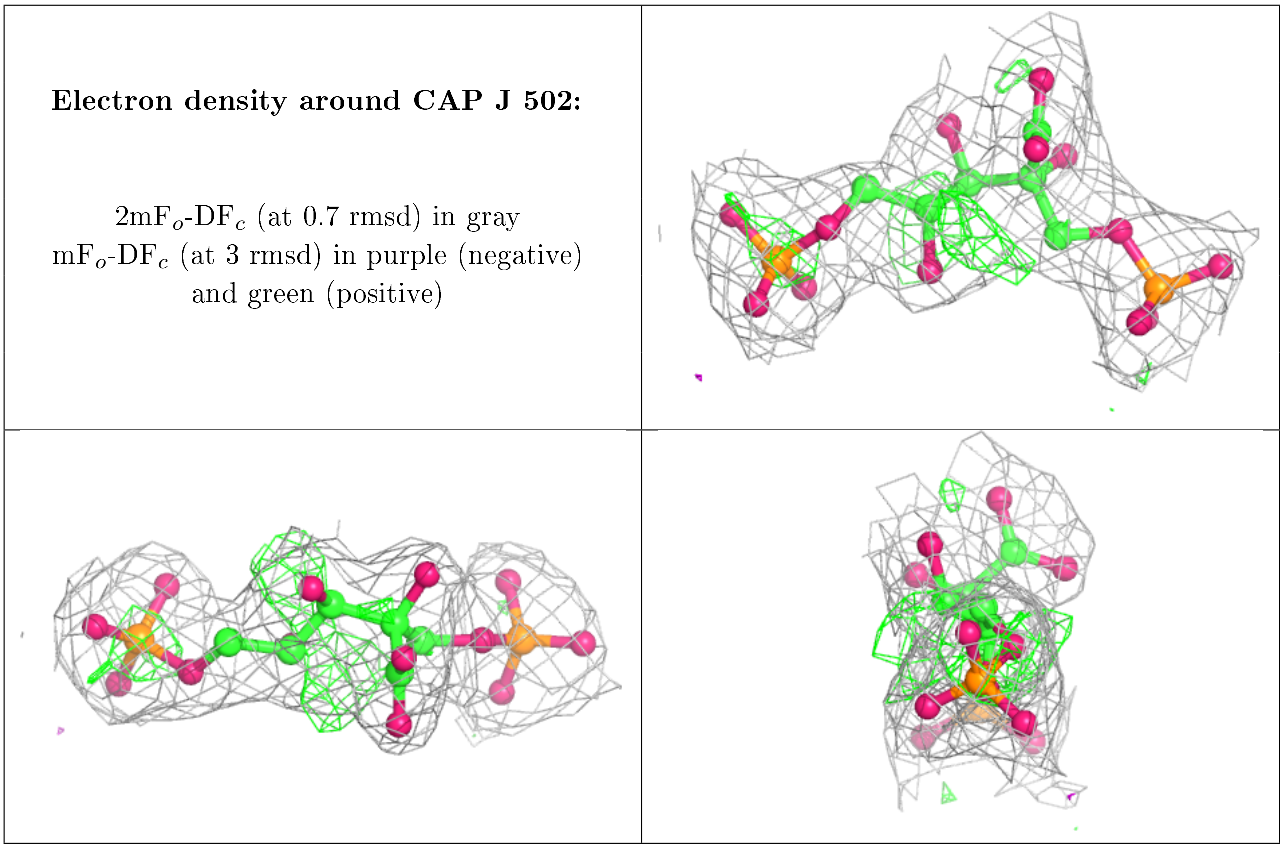
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
3	CAP	D	502	21/21	0.98	0.14	32,35,38,39	0
2	MG	D	501	1/1	0.98	0.16	31,31,31,31	0
4	EDO	B	503	4/4	0.98	0.13	31,31,31,33	0

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.

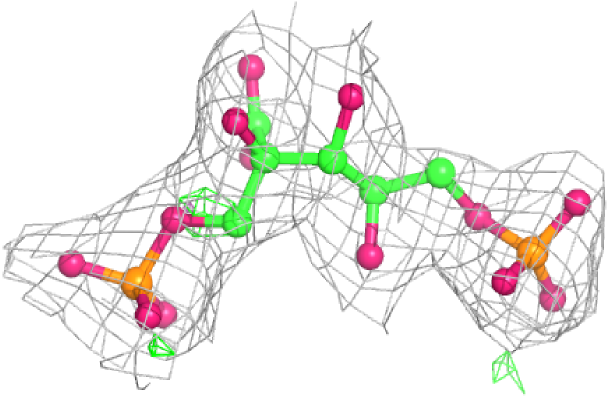
Electron density around CAP J 502:

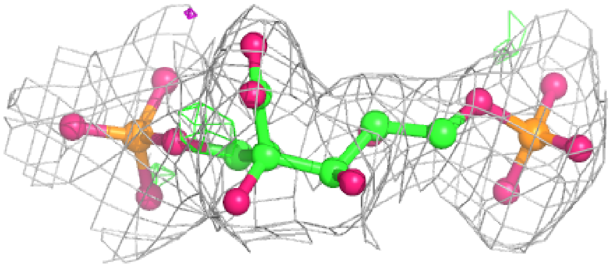
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

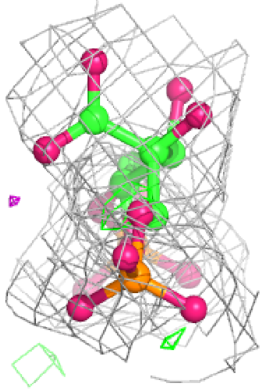


Electron density around CAP B 502:

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

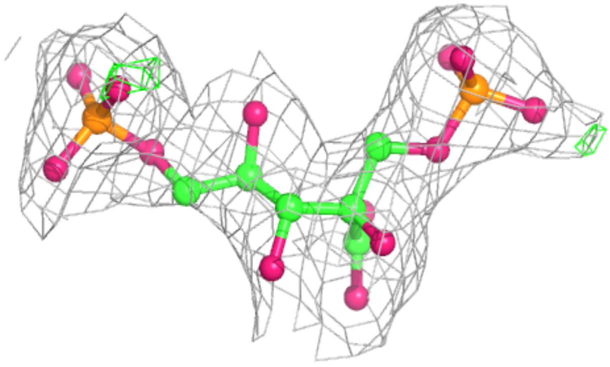


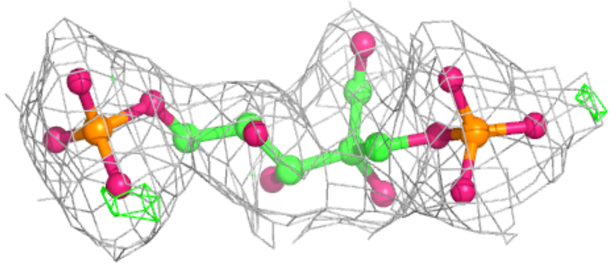


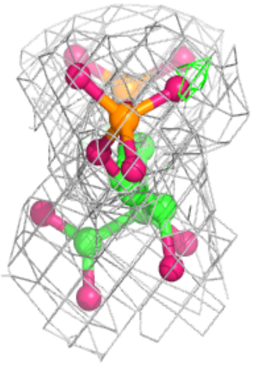


Electron density around CAP G 502:

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

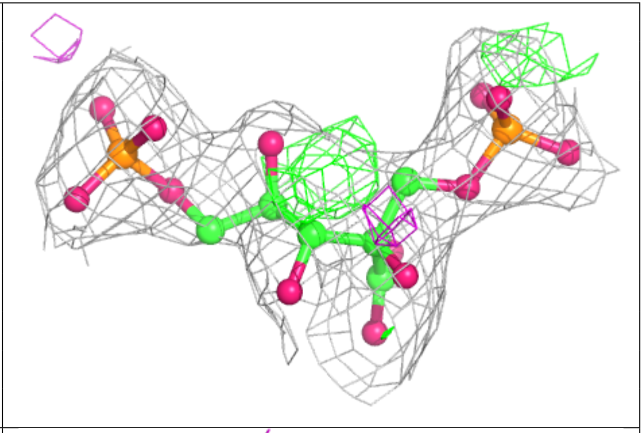


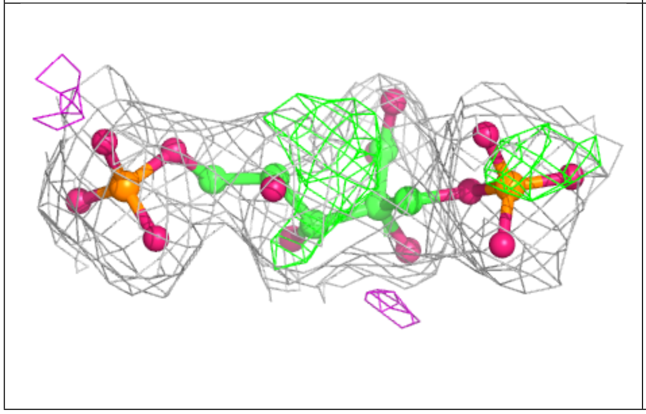


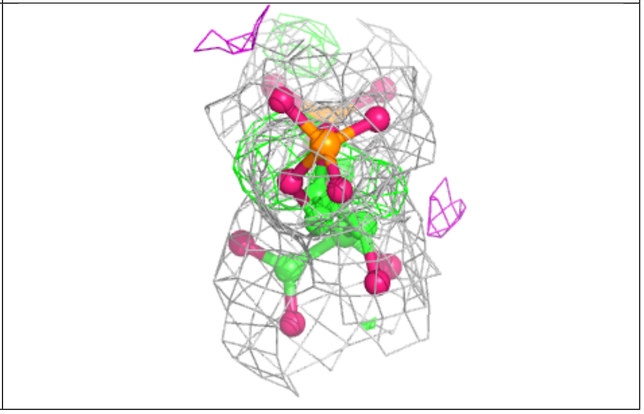


Electron density around CAP E 502:

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

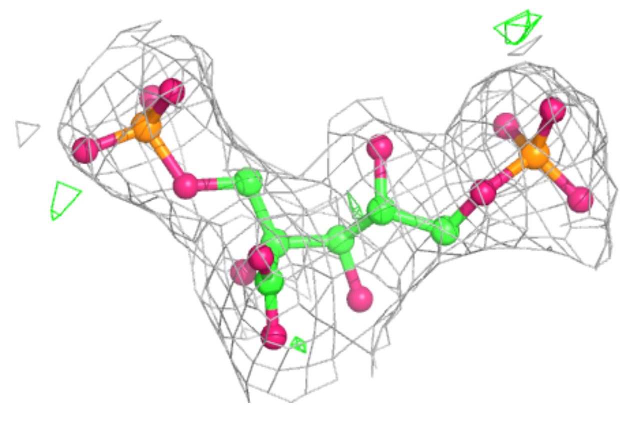


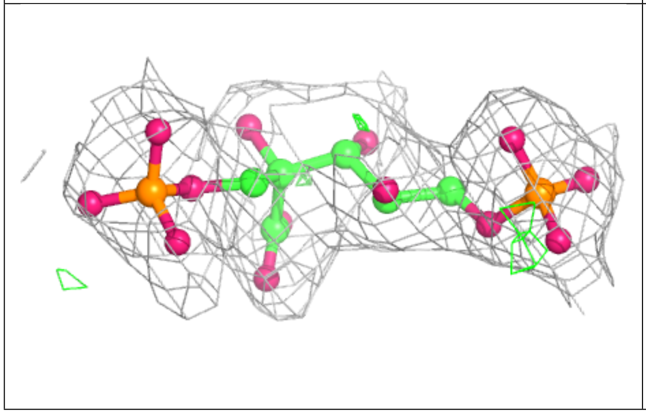


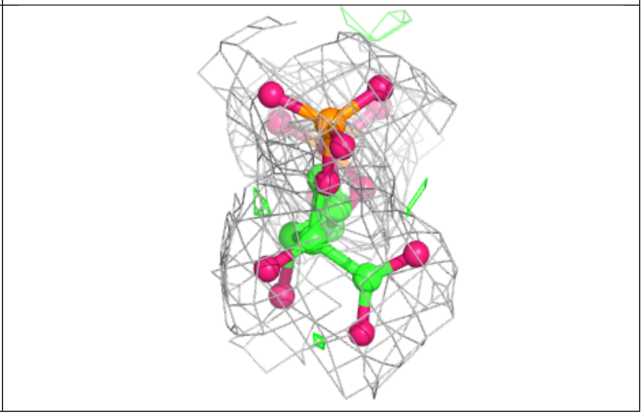


Electron density around CAP H 502:

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

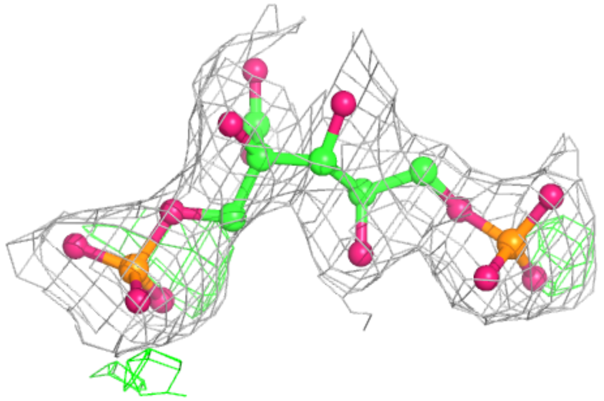


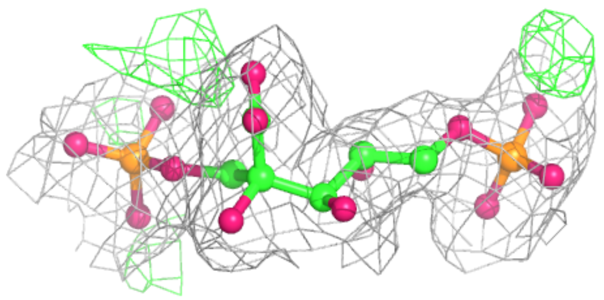


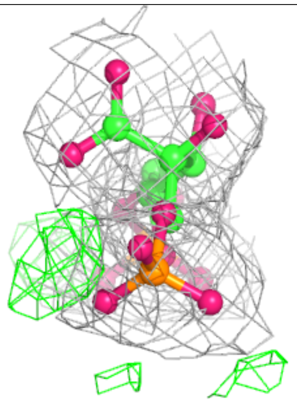


Electron density around CAP F 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

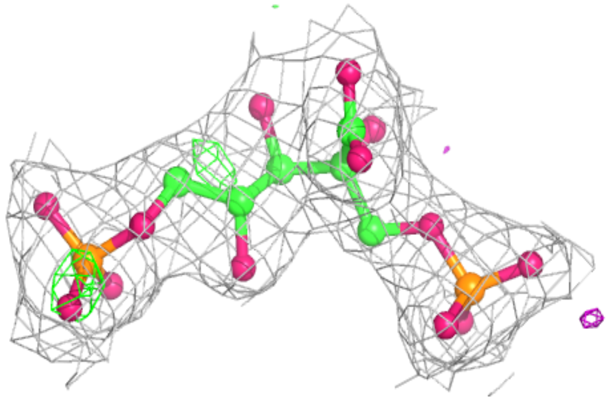


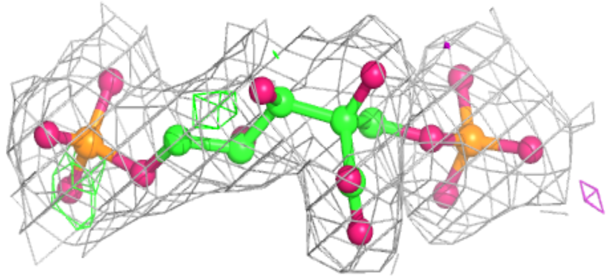


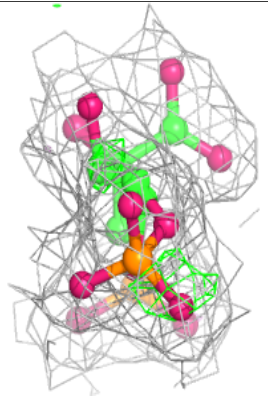


Electron density around CAP I 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

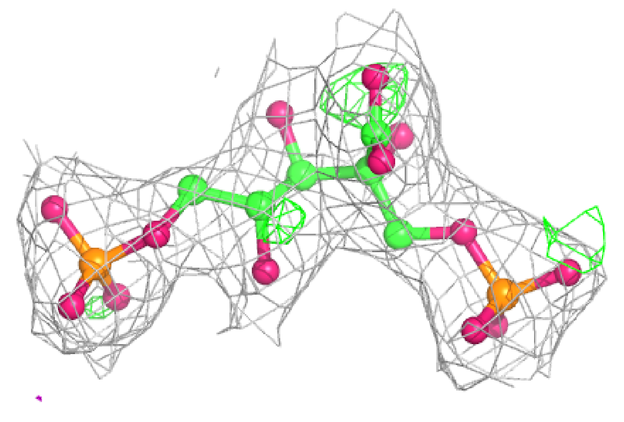


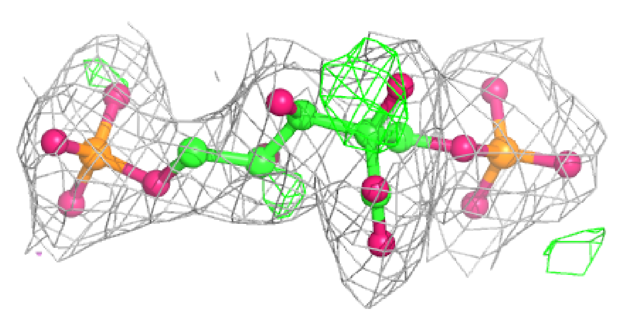


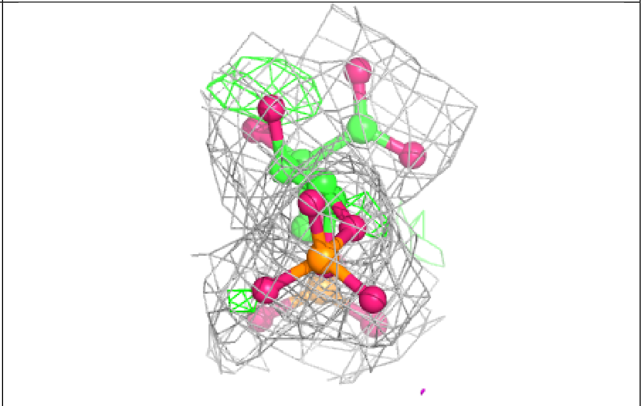


Electron density around CAP C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

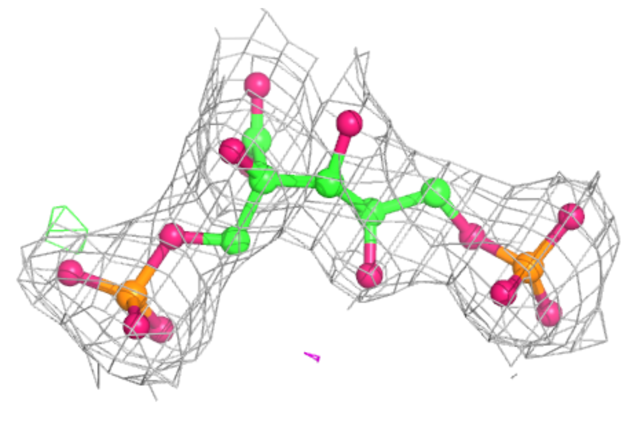


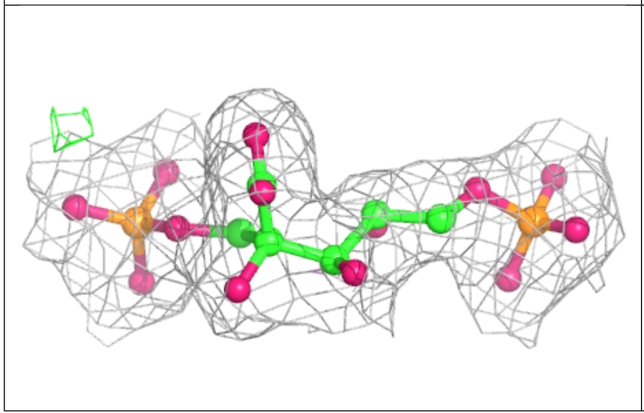


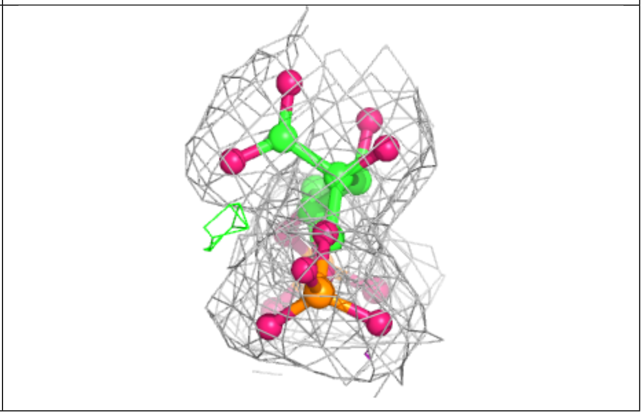


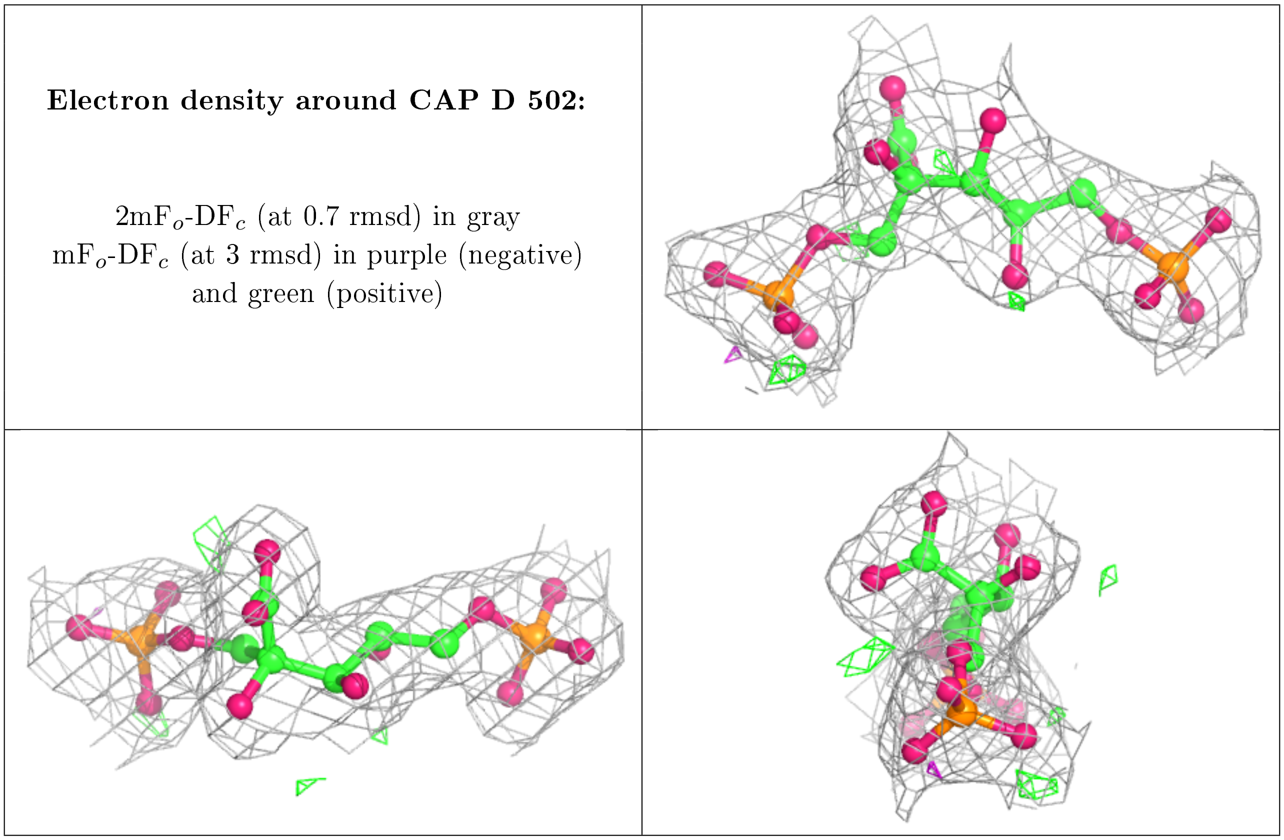
Electron density around CAP A 502:

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 502:

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

There are no such residues in this entry.