



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:19 PM GMT

PDB ID : 1IR2
Title : Crystal Structure of Activated Ribulose-1,5-bisphosphate Carboxylase/oxygenase (Rubisco) from Green alga, Chlamydomonas reinhardtii Complexed with 2-Carboxyarabinitol-1,5-bisphosphate (2-CABP)
Authors : Mizohata, E.; Matsumura, H.; Okano, Y.; Kumei, M.; Takuma, H.; Onodera, J.; Kato, K.; Shibata, N.; Inoue, T.; Yokota, A.; Kai, Y.
Deposited on : 2001-09-03
Resolution : 1.84 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

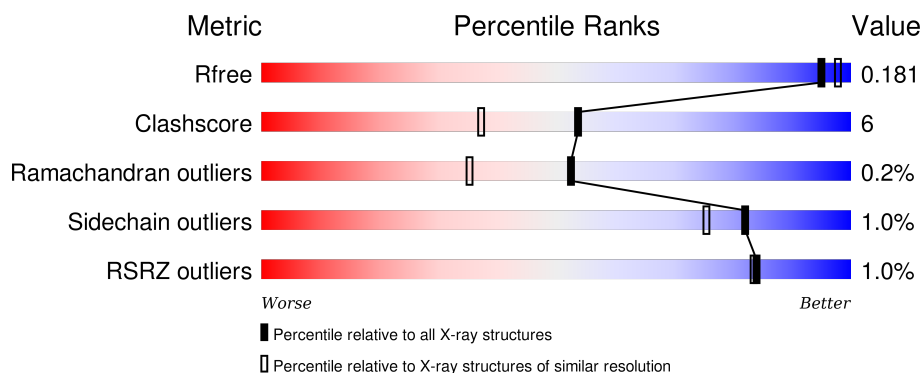
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.









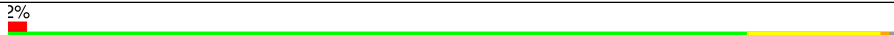
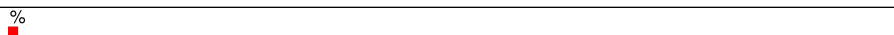
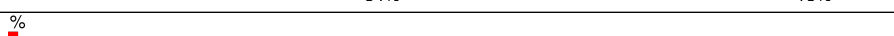
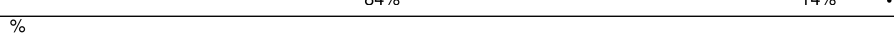
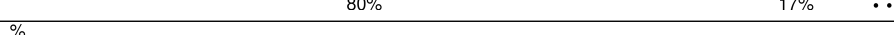
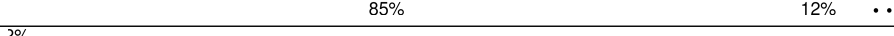













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	475	<div> <div>88%</div> <div>10% ..</div> </div>
1	B	475	<div> <div>84%</div> <div>14% .</div> </div>
1	C	475	<div> <div>84%</div> <div>13% ..</div> </div>
1	D	475	<div> <div>86%</div> <div>12% .</div> </div>
1	E	475	<div> <div>85%</div> <div>12% ..</div> </div>



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Mol	Chain	Length	Quality of chain
1	F	475	
1	G	475	
1	H	475	
1	S	475	
1	T	475	
1	U	475	
1	V	475	
1	W	475	
1	X	475	
1	Y	475	
1	Z	475	
2	1	140	
2	2	140	
2	3	140	
2	4	140	
2	5	140	
2	6	140	
2	7	140	
2	8	140	
2	I	140	
2	J	140	
2	K	140	
2	L	140	
2	M	140	
2	N	140	

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Mol	Chain	Length	Quality of chain
2	O	140	 84%16%
2	P	140	 80%19%.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	605	-	-	-	X
5	GOL	A	613	-	-	-	X
5	GOL	B	606	-	-	-	X
5	GOL	B	614	-	-	-	X
5	GOL	C	615	-	-	-	X
5	GOL	D	608	-	-	-	X
5	GOL	D	616	-	-	-	X
5	GOL	E	601	-	-	-	X
5	GOL	E	609	-	-	-	X
5	GOL	E	620	-	-	-	X
5	GOL	F	617	-	-	-	X
5	GOL	G	611	-	-	-	X
5	GOL	G	618	-	-	-	X
5	GOL	H	604	-	-	-	X
5	GOL	H	612	-	-	-	X
5	GOL	H	619	-	-	-	X
5	GOL	S	609	-	-	-	X
5	GOL	S	613	-	-	-	X
5	GOL	U	607	-	-	-	X
5	GOL	V	608	-	-	-	X
5	GOL	V	616	-	-	-	X
5	GOL	W	620	-	-	-	X
5	GOL	X	610	-	-	-	X
5	GOL	X	617	-	-	-	X
5	GOL	Y	611	-	-	-	X
5	GOL	Y	618	-	-	-	X
5	GOL	Z	604	-	-	-	X
5	GOL	Z	612	-	-	-	X
5	GOL	Z	619	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 87087 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 Large subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	B	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	C	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	D	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	E	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	F	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	G	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	H	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	S	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	T	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	U	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	V	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	W	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	X	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	Y	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	Z	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	SEE REMARK 999	UNP P00877
A	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
A	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
A	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
A	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
A	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
B	46	PRO	LEU	SEE REMARK 999	UNP P00877
B	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
B	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
B	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
B	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
B	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
C	46	PRO	LEU	SEE REMARK 999	UNP P00877
C	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
C	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
C	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
C	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
C	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
D	46	PRO	LEU	SEE REMARK 999	UNP P00877
D	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
D	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
D	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
D	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
D	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
E	46	PRO	LEU	SEE REMARK 999	UNP P00877
E	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
E	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
E	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
E	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
E	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
F	46	PRO	LEU	SEE REMARK 999	UNP P00877
F	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
F	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
F	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
F	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
F	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
G	46	PRO	LEU	SEE REMARK 999	UNP P00877
G	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
G	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
G	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
G	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
G	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
H	46	PRO	LEU	SEE REMARK 999	UNP P00877
H	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
H	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
H	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
H	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
H	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
S	46	PRO	LEU	SEE REMARK 999	UNP P00877
S	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
S	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
S	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
S	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
S	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
T	46	PRO	LEU	SEE REMARK 999	UNP P00877
T	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
T	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
T	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
T	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
T	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
U	46	PRO	LEU	SEE REMARK 999	UNP P00877
U	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
U	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
U	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
U	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
U	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
V	46	PRO	LEU	SEE REMARK 999	UNP P00877
V	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
V	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
V	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
V	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
V	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
W	46	PRO	LEU	SEE REMARK 999	UNP P00877
W	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
W	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
W	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
W	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
W	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
X	46	PRO	LEU	SEE REMARK 999	UNP P00877
X	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
X	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
X	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
X	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
X	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	46	PRO	LEU	SEE REMARK 999	UNP P00877
Y	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Y	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Y	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
Y	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Y	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Z	46	PRO	LEU	SEE REMARK 999	UNP P00877
Z	104	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Z	151	HYP	PRO	MODIFIED RESIDUE	UNP P00877
Z	201	KCX	LYS	MODIFIED RESIDUE	UNP P00877
Z	256	SMC	CYS	MODIFIED RESIDUE	UNP P00877
Z	369	SMC	CYS	MODIFIED RESIDUE	UNP P00877

- Molecule 2 is a protein called Small subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	J	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	K	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	L	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	M	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	N	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	O	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	P	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	1	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	2	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	3	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	4	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	5	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	6	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	7	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	8	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MME	MET	MODIFIED RESIDUE	UNP P08475
J	1	MME	MET	MODIFIED RESIDUE	UNP P08475
K	1	MME	MET	MODIFIED RESIDUE	UNP P08475
L	1	MME	MET	MODIFIED RESIDUE	UNP P08475
M	1	MME	MET	MODIFIED RESIDUE	UNP P08475
N	1	MME	MET	MODIFIED RESIDUE	UNP P08475
O	1	MME	MET	MODIFIED RESIDUE	UNP P08475
P	1	MME	MET	MODIFIED RESIDUE	UNP P08475
1	1	MME	MET	MODIFIED RESIDUE	UNP P08475
2	1	MME	MET	MODIFIED RESIDUE	UNP P08475
3	1	MME	MET	MODIFIED RESIDUE	UNP P08475
4	1	MME	MET	MODIFIED RESIDUE	UNP P08475
5	1	MME	MET	MODIFIED RESIDUE	UNP P08475
6	1	MME	MET	MODIFIED RESIDUE	UNP P08475
7	1	MME	MET	MODIFIED RESIDUE	UNP P08475
8	1	MME	MET	MODIFIED RESIDUE	UNP P08475

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

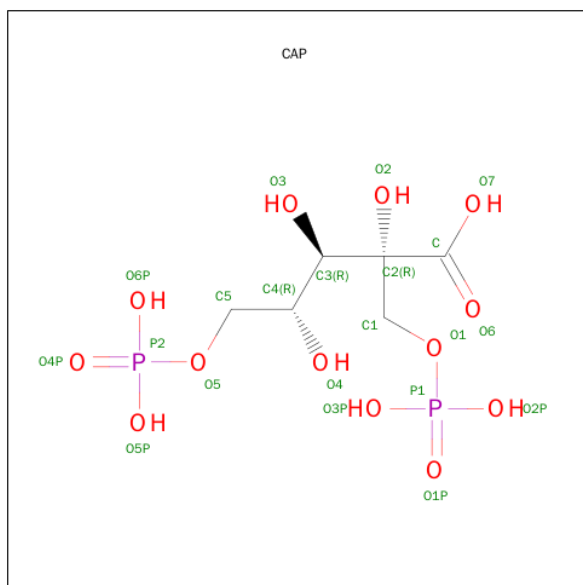
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	Z	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	T	1	Total	Mg	0	0
			1	1		
3	U	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	Y	1	Total	Mg	0	0
			1	1		
3	S	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	S	1	Total	C	O	P	0	0
			21	6	13	2		
4	T	1	Total	C	O	P	0	0
			21	6	13	2		
4	U	1	Total	C	O	P	0	0
			21	6	13	2		
4	V	1	Total	C	O	P	0	0
			21	6	13	2		
4	W	1	Total	C	O	P	0	0
			21	6	13	2		
4	X	1	Total	C	O	P	0	0
			21	6	13	2		
4	Y	1	Total	C	O	P	0	0
			21	6	13	2		
4	Z	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	F	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	W	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	Y	1	Total 6	C 3	O 3	0	0
5	Z	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0
5	V	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	Y	1	Total 6	C 3	O 3	0	0
5	Z	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	V	1	Total	C	O	0	0
			6	3	3		
5	X	1	Total	C	O	0	0
			6	3	3		
5	Y	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		
5	W	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	173	Total	O	0	0
			173	173		
6	2	173	Total	O	0	0
			173	173		
6	3	170	Total	O	0	0
			170	170		
6	4	174	Total	O	0	0
			174	174		
6	5	174	Total	O	0	0
			174	174		
6	6	146	Total	O	0	0
			146	146		
6	7	184	Total	O	0	0
			184	184		
6	8	185	Total	O	0	0
			185	185		
6	A	459	Total	O	0	0
			459	459		
6	B	406	Total	O	0	0
			406	406		
6	C	478	Total	O	0	0
			478	478		
6	D	480	Total	O	0	0
			480	480		
6	E	463	Total	O	0	0
			463	463		
6	F	450	Total	O	0	0
			450	450		

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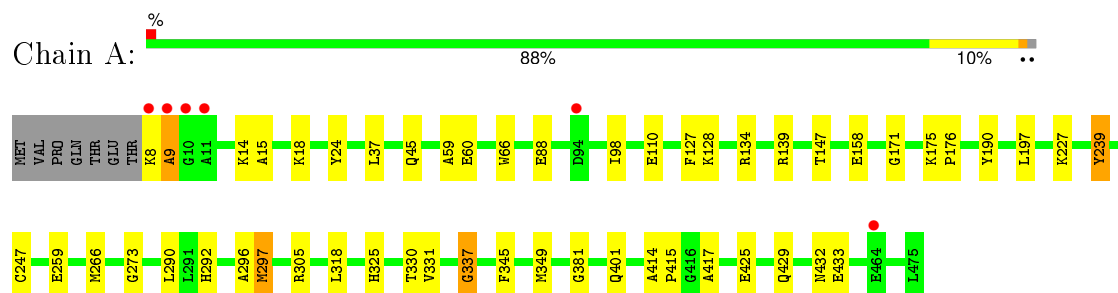
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	466	Total 466	O 466	0	0
6	H	452	Total 452	O 452	0	0
6	I	172	Total 172	O 172	0	0
6	J	170	Total 170	O 170	0	0
6	K	187	Total 187	O 187	0	0
6	L	186	Total 186	O 186	0	0
6	M	181	Total 181	O 181	0	0
6	N	186	Total 186	O 186	0	0
6	O	179	Total 179	O 179	0	0
6	P	200	Total 200	O 200	0	0
6	S	425	Total 425	O 425	0	0
6	T	426	Total 426	O 426	0	0
6	U	427	Total 427	O 427	0	0
6	V	456	Total 456	O 456	0	0
6	W	421	Total 421	O 421	0	0
6	X	450	Total 450	O 450	0	0
6	Y	426	Total 426	O 426	0	0
6	Z	474	Total 474	O 474	0	0

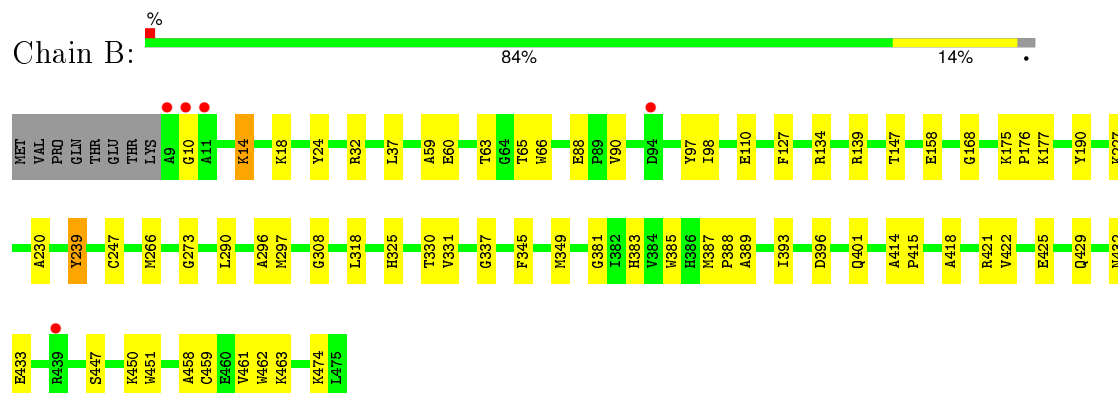
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

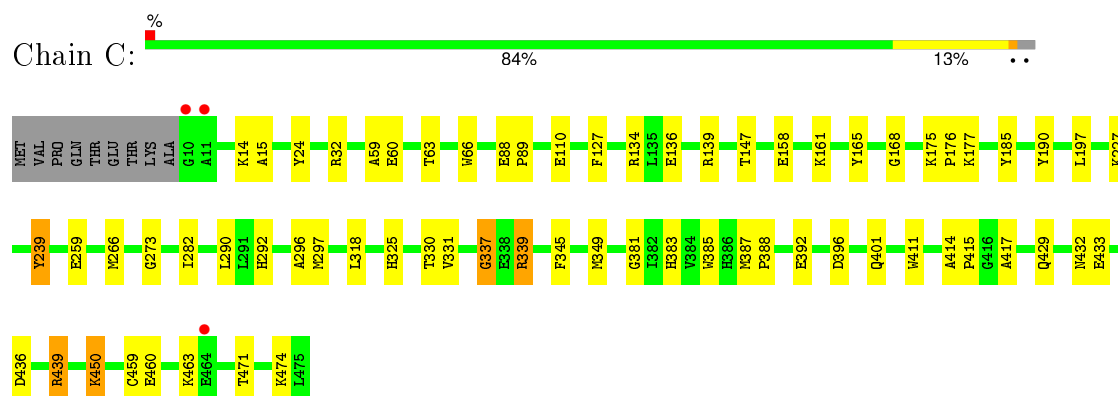
- Molecule 1: Large subunit of Rubisco



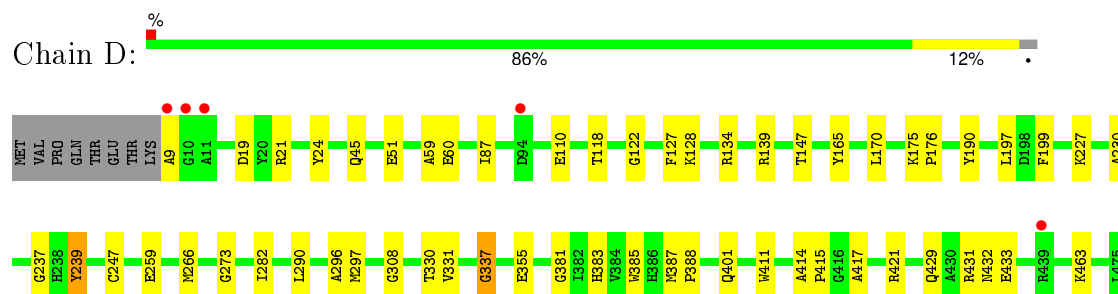
- Molecule 1: Large subunit of Rubisco



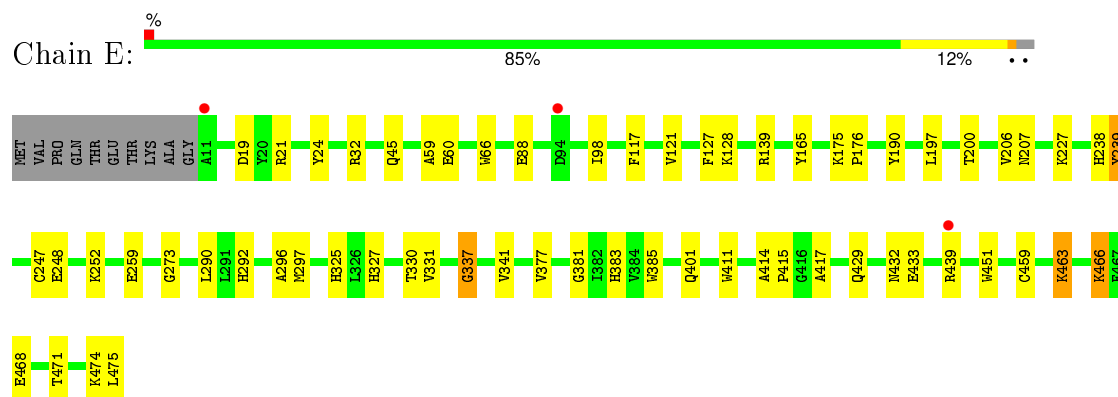
- Molecule 1: Large subunit of Rubisco



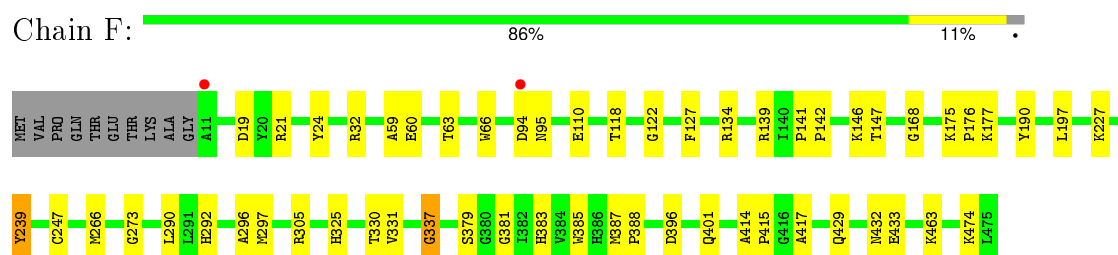
- Molecule 1: Large subunit of Rubisco



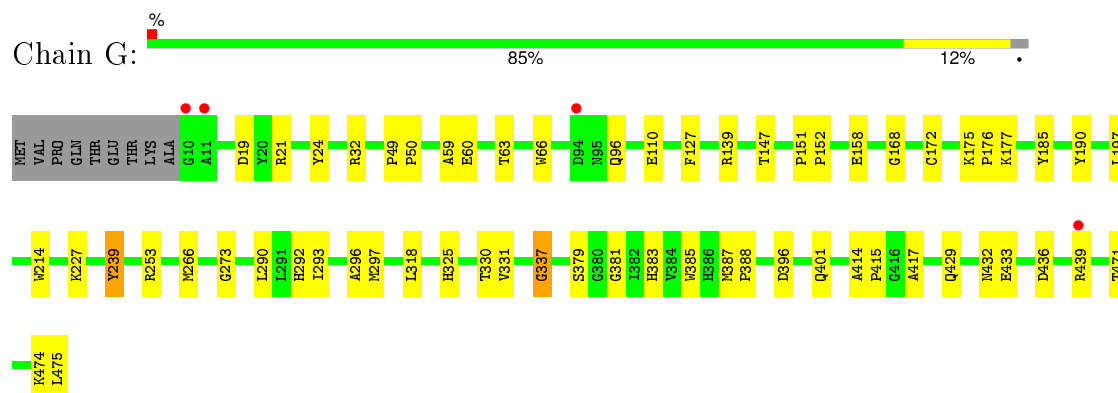
- Molecule 1: Large subunit of Rubisco



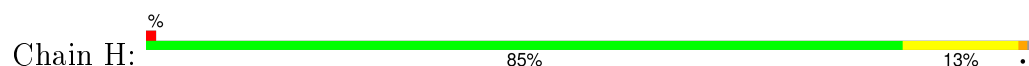
- Molecule 1: Large subunit of Rubisco

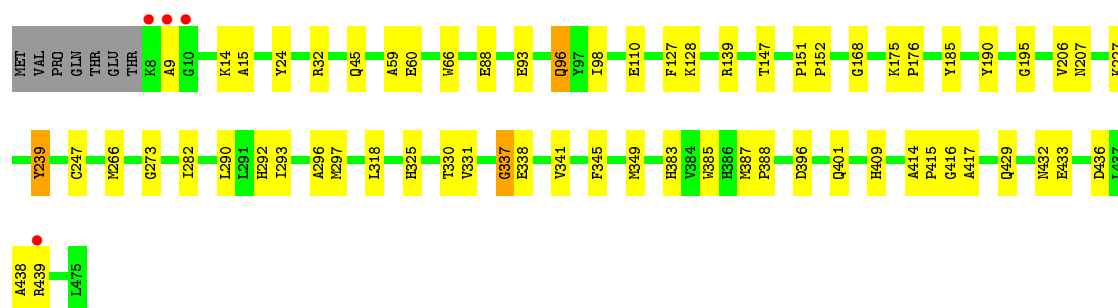


- Molecule 1: Large subunit of Rubisco



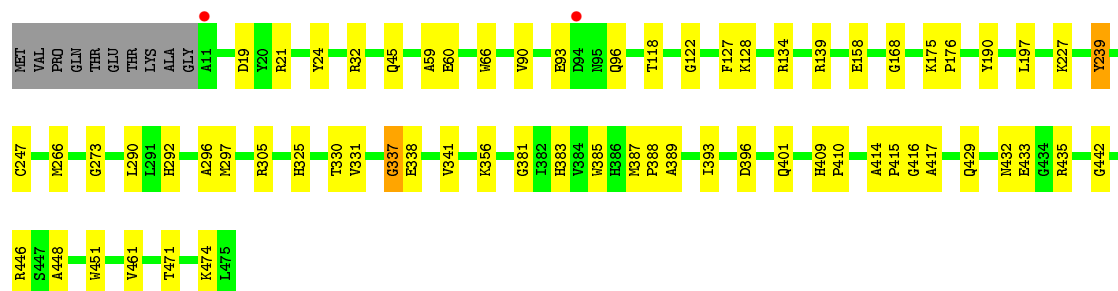
- Molecule 1: Large subunit of Rubisco





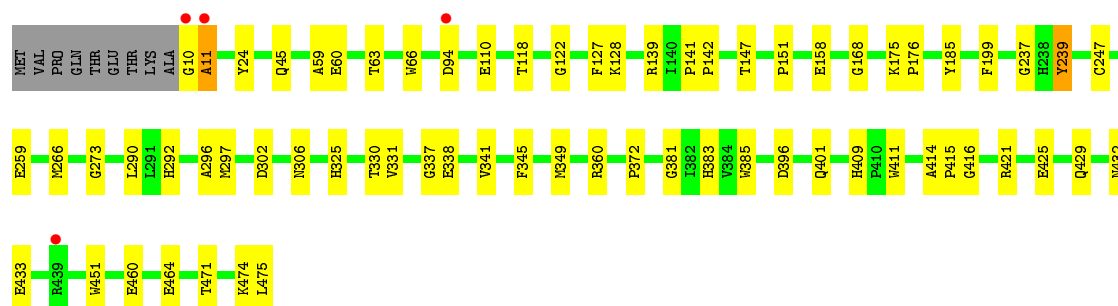
- Molecule 1: Large subunit of Rubisco

Chain S: 84% 13%



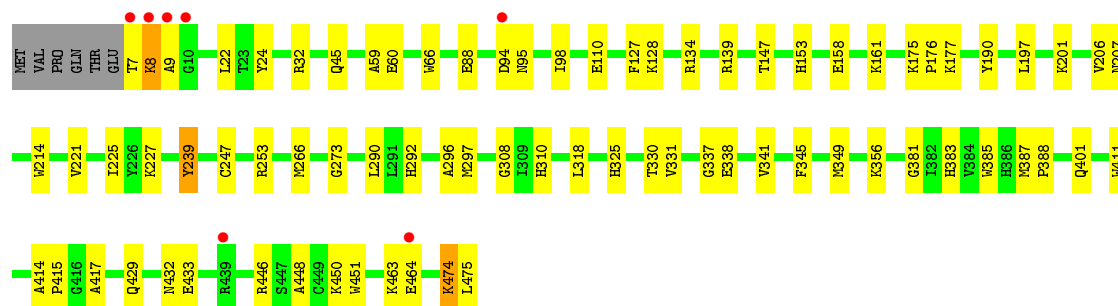
- Molecule 1: Large subunit of Rubisco

Chain T: 84% 14%

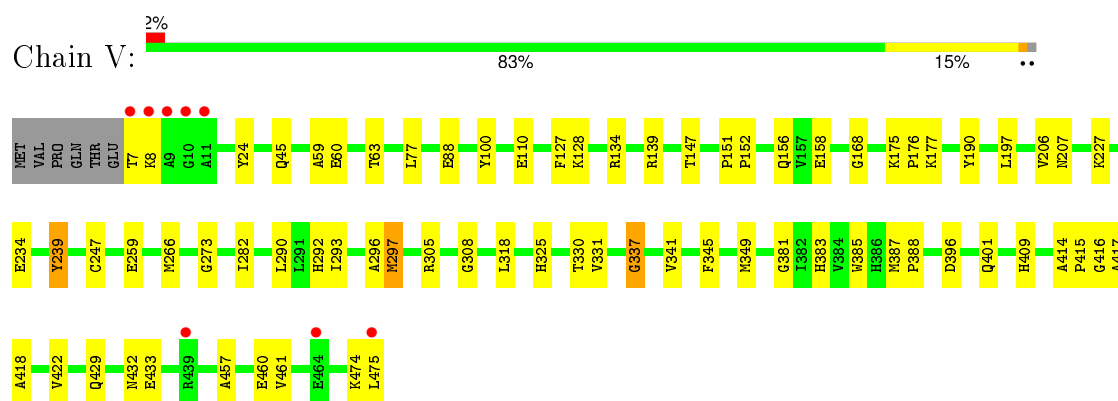


- Molecule 1: Large subunit of Rubisco

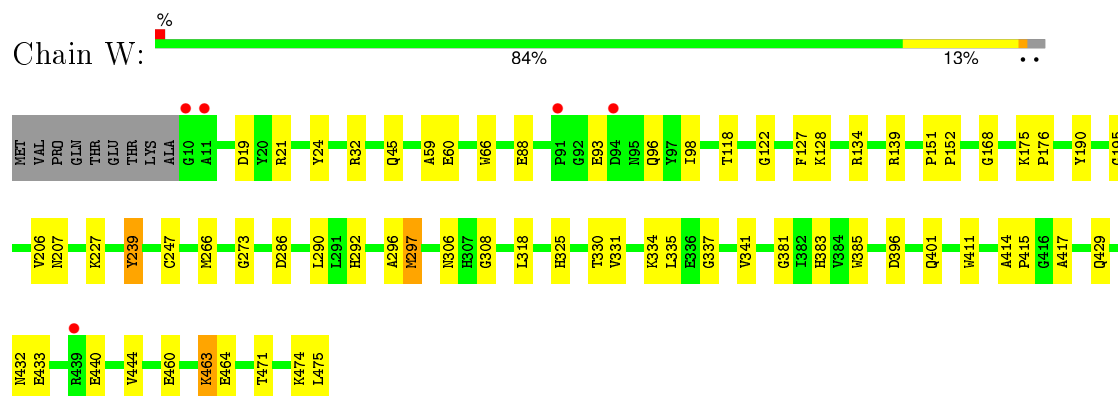
Chain U: 83% 16%



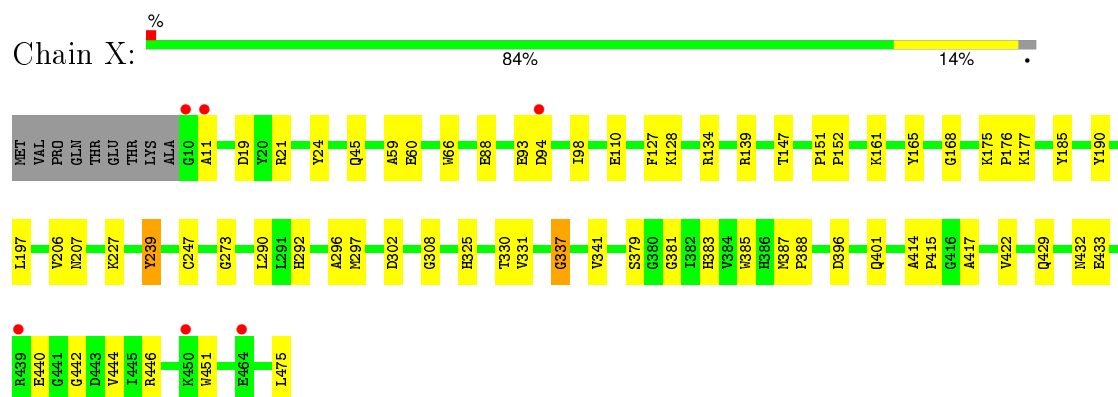
- Molecule 1: Large subunit of Rubisco



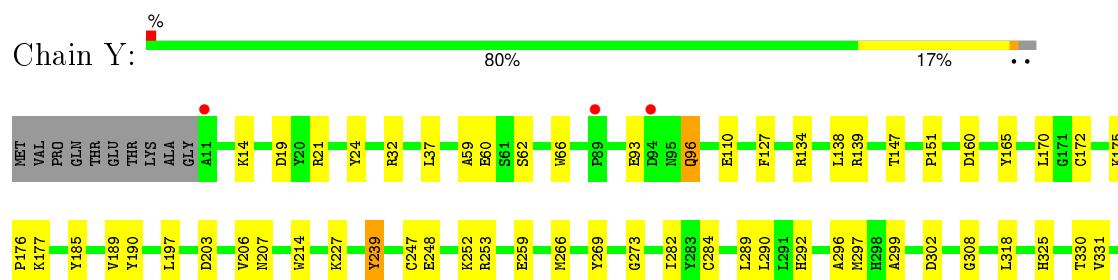
- Molecule 1: Large subunit of Rubisco



- Molecule 1: Large subunit of Rubisco

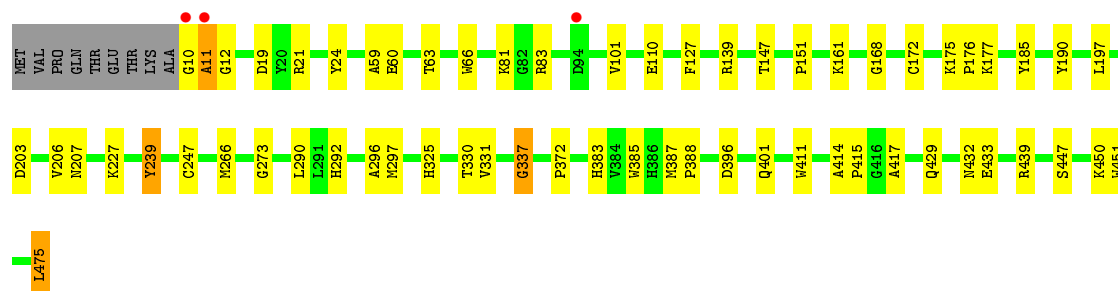
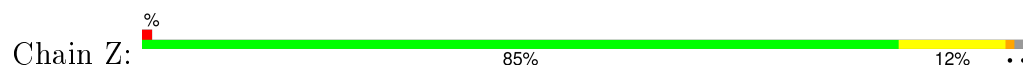


- Molecule 1: Large subunit of Rubisco

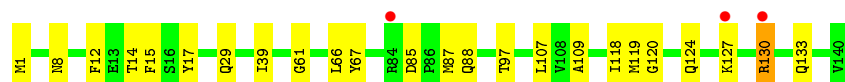
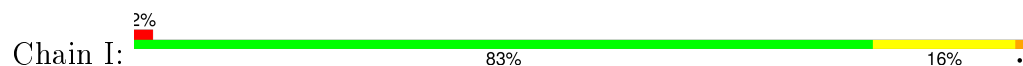




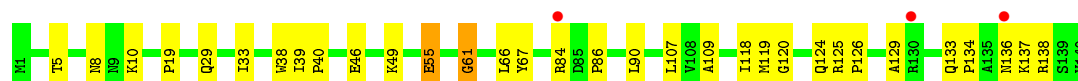
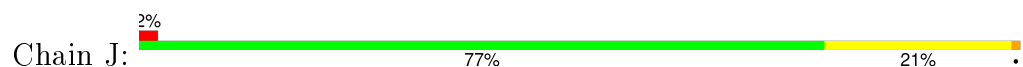
- Molecule 1: Large subunit of Rubisco



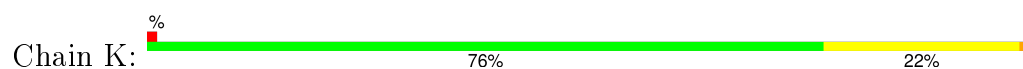
- Molecule 2: Small subunit of Rubisco



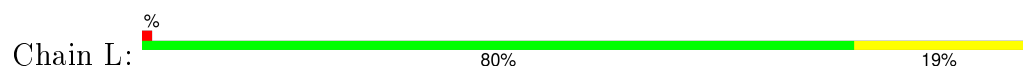
- Molecule 2: Small subunit of Rubisco



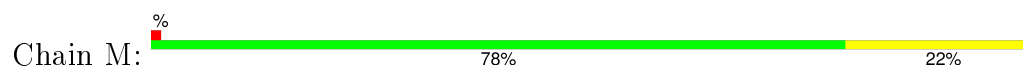
- Molecule 2: Small subunit of Rubisco

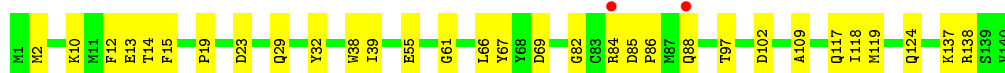


- Molecule 2: Small subunit of Rubisco

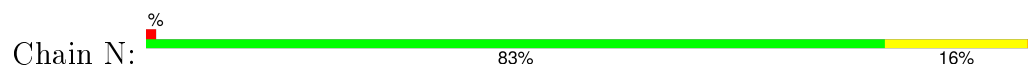


- Molecule 2: Small subunit of Rubisco

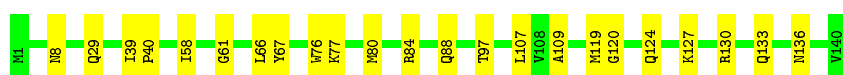
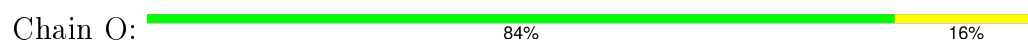




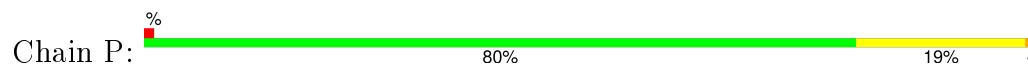
- Molecule 2: Small subunit of Rubisco



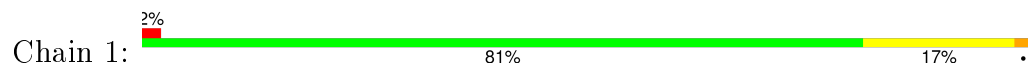
- Molecule 2: Small subunit of Rubisco



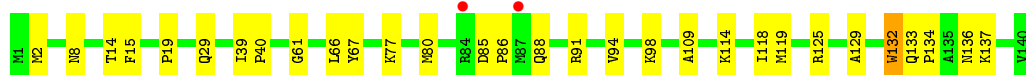
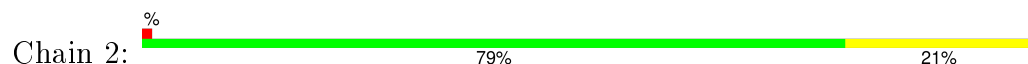
- Molecule 2: Small subunit of Rubisco



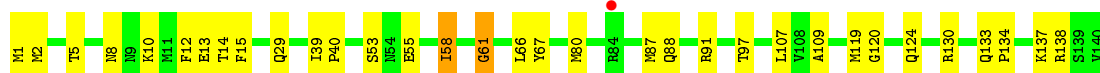
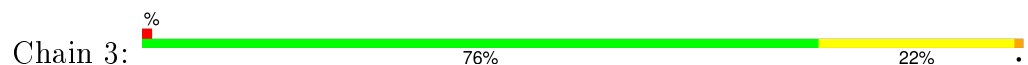
- Molecule 2: Small subunit of Rubisco



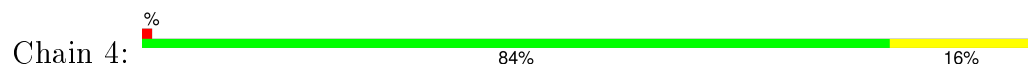
- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.17Å 174.75Å 222.27Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	39.89 – 1.84 40.02 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.89-1.84) 90.7 (40.02-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.84Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.152 , 0.181 0.152 , 0.181	Depositor DCC
R_{free} test set	37921 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 763081 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	87087	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, CAP, HYP, MME, SMC, 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	0.31	0/3684	0.60	0/4978
1	B	0.30	0/3675	0.61	0/4967
1	C	0.31	0/3670	0.61	0/4960
1	D	0.31	0/3675	0.61	0/4967
1	E	0.31	0/3666	0.62	0/4955
1	F	0.30	0/3666	0.60	0/4955
1	G	0.31	0/3670	0.61	0/4960
1	H	0.31	0/3684	0.62	0/4978
1	S	0.30	0/3666	0.61	0/4955
1	T	0.31	0/3670	0.61	0/4960
1	U	0.31	0/3691	0.61	0/4988
1	V	0.31	0/3691	0.62	0/4988
1	W	0.30	0/3670	0.60	0/4960
1	X	0.31	0/3670	0.60	0/4960
1	Y	0.31	0/3666	0.61	0/4955
1	Z	0.31	0/3670	0.61	0/4960
2	1	0.31	0/1169	0.60	1/1588 (0.1%)
2	2	0.30	0/1169	0.59	1/1588 (0.1%)
2	3	0.32	0/1169	0.60	1/1588 (0.1%)
2	4	0.32	0/1169	0.59	1/1588 (0.1%)
2	5	0.31	0/1169	0.61	1/1588 (0.1%)
2	6	0.31	0/1169	0.59	1/1588 (0.1%)
2	7	0.32	0/1169	0.60	1/1588 (0.1%)
2	8	0.32	0/1169	0.61	1/1588 (0.1%)
2	I	0.31	0/1169	0.59	1/1588 (0.1%)
2	J	0.30	0/1169	0.59	1/1588 (0.1%)
2	K	0.31	0/1169	0.60	1/1588 (0.1%)
2	L	0.32	0/1169	0.60	1/1588 (0.1%)
2	M	0.31	0/1169	0.60	1/1588 (0.1%)
2	N	0.31	0/1169	0.59	1/1588 (0.1%)
2	O	0.32	0/1169	0.60	1/1588 (0.1%)
2	P	0.32	0/1169	0.60	1/1588 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.31	0/77488	0.61	16/104854 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	61	GLY	N-CA-C	-6.03	98.03	113.10
2	M	61	GLY	N-CA-C	-6.02	98.05	113.10
2	J	61	GLY	N-CA-C	-5.99	98.13	113.10
2	6	61	GLY	N-CA-C	-5.97	98.17	113.10
2	L	61	GLY	N-CA-C	-5.96	98.19	113.10

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	3646	0	3559	36	0
1	B	3637	0	3546	50	0
1	C	3632	0	3541	48	0
1	D	3637	0	3546	48	0
1	E	3628	0	3538	41	0
1	F	3628	0	3538	39	0
1	G	3632	0	3541	37	0
1	H	3646	0	3559	42	0
1	S	3628	0	3538	47	0
1	T	3632	0	3541	44	0
1	U	3653	0	3566	65	0
1	V	3653	0	3566	47	0
1	W	3632	0	3541	46	0
1	X	3632	0	3541	39	0
1	Y	3628	0	3538	57	0
1	Z	3632	0	3541	44	0
2	1	1145	0	1119	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1145	0	1119	22	0
2	3	1145	0	1119	33	0
2	4	1145	0	1119	19	0
2	5	1145	0	1119	15	0
2	6	1145	0	1119	23	0
2	7	1145	0	1119	18	0
2	8	1145	0	1119	27	0
2	I	1145	0	1119	19	0
2	J	1145	0	1119	25	0
2	K	1145	0	1119	30	0
2	L	1145	0	1119	25	0
2	M	1145	0	1119	30	0
2	N	1145	0	1119	23	0
2	O	1145	0	1119	16	0
2	P	1145	0	1119	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	8	0	0
4	C	21	0	8	0	0
4	D	21	0	7	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	8	0	0
4	H	21	0	7	0	0
4	S	21	0	7	0	0
4	T	21	0	7	0	0
4	U	21	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	21	0	7	0	0
4	W	21	0	8	0	0
4	X	21	0	8	0	0
4	Y	21	0	8	0	0
4	Z	21	0	8	0	0
5	A	12	0	16	1	0
5	B	18	0	24	2	0
5	C	12	0	16	1	0
5	D	12	0	16	1	0
5	E	18	0	24	0	0
5	F	12	0	16	1	0
5	G	18	0	24	0	0
5	H	18	0	24	1	0
5	S	18	0	24	0	0
5	T	12	0	16	0	0
5	U	12	0	16	0	0
5	V	12	0	16	1	0
5	W	12	0	16	1	0
5	X	18	0	24	0	0
5	Y	18	0	24	1	0
5	Z	18	0	24	0	0
6	1	173	0	0	2	0
6	2	173	0	0	1	0
6	3	170	0	0	3	0
6	4	174	0	0	2	0
6	5	174	0	0	0	0
6	6	146	0	0	2	0
6	7	184	0	0	3	0
6	8	185	0	0	1	0
6	A	459	0	0	1	0
6	B	406	0	0	4	0
6	C	478	0	0	2	0
6	D	480	0	0	6	0
6	E	463	0	0	3	0
6	F	450	0	0	5	0
6	G	466	0	0	3	0
6	H	452	0	0	3	0
6	I	172	0	0	3	0
6	J	170	0	0	3	0
6	K	187	0	0	3	0
6	L	186	0	0	5	0
6	M	181	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	186	0	0	2	0
6	O	179	0	0	0	0
6	P	200	0	0	3	0
6	S	425	0	0	5	0
6	T	426	0	0	5	0
6	U	427	0	0	7	0
6	V	456	0	0	3	0
6	W	421	0	0	6	0
6	X	450	0	0	2	0
6	Y	426	0	0	7	0
6	Z	474	0	0	5	0
All	All	87087	0	75085	975	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 6.

The worst 5 of 975 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:U:8:LYS:HD2	2:8:84:ARG:HH11	1.07	1.10
1:U:8:LYS:HG2	1:U:9:ALA:H	1.00	1.08
1:A:247:CYS:HG	1:E:247:CYS:HG	1.07	0.96
1:U:8:LYS:HG2	1:U:9:ALA:N	1.84	0.92
1:D:247:CYS:HG	1:H:247:CYS:HG	1.11	0.92

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	461/475 (97%)	444 (96%)	15 (3%)	2 (0%)	39 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/475 (97%)	443 (96%)	16 (4%)	1 (0%)	52	35
1	C	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	52	35
1	D	460/475 (97%)	445 (97%)	14 (3%)	1 (0%)	52	35
1	E	458/475 (96%)	442 (96%)	15 (3%)	1 (0%)	52	35
1	F	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	52	35
1	G	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	52	35
1	H	461/475 (97%)	448 (97%)	11 (2%)	2 (0%)	39	22
1	S	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	52	35
1	T	459/475 (97%)	445 (97%)	12 (3%)	2 (0%)	39	22
1	U	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	39	22
1	V	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	39	22
1	W	459/475 (97%)	443 (96%)	15 (3%)	1 (0%)	52	35
1	X	459/475 (97%)	444 (97%)	13 (3%)	2 (0%)	39	22
1	Y	458/475 (96%)	444 (97%)	13 (3%)	1 (0%)	52	35
1	Z	459/475 (97%)	442 (96%)	15 (3%)	2 (0%)	39	22
2	1	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	2	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	3	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	4	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	5	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	6	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	7	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	8	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	I	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	J	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	K	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
2	L	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	M	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	O	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	P	138/140 (99%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9560/9840 (97%)	9177 (96%)	360 (4%)	23 (0%)	52 35

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	T	11	ALA
1	U	8	LYS
1	Z	11	ALA
1	X	11	ALA

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	369/376 (98%)	367 (100%)	2 (0%)	92 89
1	B	368/376 (98%)	366 (100%)	2 (0%)	92 89
1	C	368/376 (98%)	363 (99%)	5 (1%)	74 63
1	D	368/376 (98%)	366 (100%)	2 (0%)	92 89
1	E	368/376 (98%)	364 (99%)	4 (1%)	80 72
1	F	368/376 (98%)	367 (100%)	1 (0%)	94 94
1	G	368/376 (98%)	363 (99%)	5 (1%)	74 63
1	H	369/376 (98%)	366 (99%)	3 (1%)	86 81
1	S	368/376 (98%)	367 (100%)	1 (0%)	94 94
1	T	368/376 (98%)	365 (99%)	3 (1%)	86 81
1	U	370/376 (98%)	367 (99%)	3 (1%)	86 81
1	V	370/376 (98%)	367 (99%)	3 (1%)	86 81
1	W	368/376 (98%)	364 (99%)	4 (1%)	80 72
1	X	368/376 (98%)	364 (99%)	4 (1%)	80 72
1	Y	368/376 (98%)	364 (99%)	4 (1%)	80 72
1	Z	368/376 (98%)	363 (99%)	5 (1%)	74 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	2	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	3	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	4	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	5	123/123 (100%)	122 (99%)	1 (1%)	86	81
2	6	123/123 (100%)	122 (99%)	1 (1%)	86	81
2	7	123/123 (100%)	122 (99%)	1 (1%)	86	81
2	8	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	I	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	J	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	K	123/123 (100%)	120 (98%)	3 (2%)	57	39
2	L	123/123 (100%)	120 (98%)	3 (2%)	57	39
2	M	123/123 (100%)	121 (98%)	2 (2%)	70	57
2	N	123/123 (100%)	122 (99%)	1 (1%)	86	81
2	O	123/123 (100%)	122 (99%)	1 (1%)	86	81
2	P	123/123 (100%)	121 (98%)	2 (2%)	70	57
All	All	7862/7984 (98%)	7782 (99%)	80 (1%)	82	75

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	185	TYR
1	T	185	TYR
1	Z	172	CYS
1	H	239	TYR
1	S	239	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	88	GLN
2	1	133	GLN
2	7	88	GLN
2	P	124	GLN
2	1	8	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

96 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	$\# Z > 2$
2	MME	1	1	2	7,8,9	1.86	1 (14%)	4,8,10	0.93	0
2	MME	2	1	2	7,8,9	1.83	1 (14%)	4,8,10	0.96	0
2	MME	3	1	2	7,8,9	1.86	1 (14%)	4,8,10	1.02	0
2	MME	4	1	2	7,8,9	1.87	1 (14%)	4,8,10	0.99	0
2	MME	5	1	2	7,8,9	1.84	1 (14%)	4,8,10	1.01	0
2	MME	6	1	2	7,8,9	1.86	1 (14%)	4,8,10	0.95	0
2	MME	7	1	2	7,8,9	1.85	1 (14%)	4,8,10	0.96	0
2	MME	8	1	2	7,8,9	1.86	1 (14%)	4,8,10	1.03	0
1	HYP	A	104	1	7,8,9	0.88	0	5,10,12	1.76	2 (40%)
1	HYP	A	151	1	7,8,9	0.89	0	5,10,12	1.43	1 (20%)
1	KCX	A	201	1,3	7,11,12	0.83	0	7,12,14	0.96	0
1	SMC	A	256	1	5,6,7	0.42	0	2,6,8	1.45	1 (50%)
1	SMC	A	369	1	5,6,7	0.62	0	2,6,8	1.04	0
1	HYP	B	104	1	7,8,9	0.90	0	5,10,12	1.60	1 (20%)
1	HYP	B	151	1	7,8,9	0.91	0	5,10,12	1.44	1 (20%)
1	KCX	B	201	1,3	7,11,12	0.62	0	7,12,14	0.92	0
1	SMC	B	256	1	5,6,7	0.55	0	2,6,8	1.53	0
1	SMC	B	369	1	5,6,7	0.56	0	2,6,8	1.01	0
1	HYP	C	104	1	7,8,9	0.92	0	5,10,12	1.56	1 (20%)
1	HYP	C	151	1	7,8,9	0.85	0	5,10,12	1.43	1 (20%)
1	KCX	C	201	1,3	7,11,12	0.80	0	7,12,14	1.00	0
1	SMC	C	256	1	5,6,7	0.49	0	2,6,8	1.48	1 (50%)
1	SMC	C	369	1	5,6,7	0.46	0	2,6,8	1.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	D	104	1	7,8,9	0.91	0	5,10,12	1.60	1 (20%)
1	HYP	D	151	1	7,8,9	0.92	0	5,10,12	1.43	1 (20%)
1	KCX	D	201	1,3	7,11,12	0.70	0	7,12,14	0.95	0
1	SMC	D	256	1	5,6,7	0.52	0	2,6,8	1.36	0
1	SMC	D	369	1	5,6,7	0.49	0	2,6,8	1.33	0
1	HYP	E	104	1	7,8,9	0.92	0	5,10,12	1.57	1 (20%)
1	HYP	E	151	1	7,8,9	0.93	0	5,10,12	1.39	1 (20%)
1	KCX	E	201	1,3	7,11,12	0.90	0	7,12,14	1.01	0
1	SMC	E	256	1	5,6,7	0.56	0	2,6,8	1.58	0
1	SMC	E	369	1	5,6,7	0.48	0	2,6,8	1.18	0
1	HYP	F	104	1	7,8,9	0.88	0	5,10,12	1.71	1 (20%)
1	HYP	F	151	1	7,8,9	0.85	0	5,10,12	1.39	1 (20%)
1	KCX	F	201	1,3	7,11,12	0.83	0	7,12,14	0.96	0
1	SMC	F	256	1	5,6,7	0.45	0	2,6,8	1.51	0
1	SMC	F	369	1	5,6,7	0.54	0	2,6,8	1.02	0
1	HYP	G	104	1	7,8,9	0.93	0	5,10,12	1.69	1 (20%)
1	HYP	G	151	1	7,8,9	0.94	0	5,10,12	1.36	1 (20%)
1	KCX	G	201	1,3	7,11,12	0.71	0	7,12,14	0.98	0
1	SMC	G	256	1	5,6,7	0.48	0	2,6,8	1.51	1 (50%)
1	SMC	G	369	1	5,6,7	0.46	0	2,6,8	1.15	0
1	HYP	H	104	1	7,8,9	0.88	0	5,10,12	1.68	1 (20%)
1	HYP	H	151	1	7,8,9	0.85	0	5,10,12	1.45	1 (20%)
1	KCX	H	201	1,3	7,11,12	0.91	0	7,12,14	1.09	0
1	SMC	H	256	1	5,6,7	0.47	0	2,6,8	1.45	0
1	SMC	H	369	1	5,6,7	0.54	0	2,6,8	1.00	0
2	MME	I	1	2	7,8,9	1.85	1 (14%)	4,8,10	0.93	0
2	MME	J	1	2	7,8,9	1.86	1 (14%)	4,8,10	1.01	0
2	MME	K	1	2	7,8,9	1.85	1 (14%)	4,8,10	0.92	0
2	MME	L	1	2	7,8,9	1.86	1 (14%)	4,8,10	0.96	0
2	MME	M	1	2	7,8,9	1.84	1 (14%)	4,8,10	0.99	0
2	MME	N	1	2	7,8,9	1.85	1 (14%)	4,8,10	1.07	0
2	MME	O	1	2	7,8,9	1.84	1 (14%)	4,8,10	0.97	0
2	MME	P	1	2	7,8,9	1.85	1 (14%)	4,8,10	1.09	0
1	HYP	S	104	1	7,8,9	0.87	0	5,10,12	1.71	1 (20%)
1	HYP	S	151	1	7,8,9	0.93	0	5,10,12	1.42	1 (20%)
1	KCX	S	201	1,3	7,11,12	0.73	0	7,12,14	1.01	0
1	SMC	S	256	1	5,6,7	0.50	0	2,6,8	1.52	0
1	SMC	S	369	1	5,6,7	0.48	0	2,6,8	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	T	104	1	7,8,9	0.89	0	5,10,12	1.57	1 (20%)
1	HYP	T	151	1	7,8,9	0.88	0	5,10,12	1.38	1 (20%)
1	KCX	T	201	1,3	7,11,12	0.89	0	7,12,14	1.02	0
1	SMC	T	256	1	5,6,7	0.55	0	2,6,8	1.67	1 (50%)
1	SMC	T	369	1	5,6,7	0.58	0	2,6,8	1.07	0
1	HYP	U	104	1	7,8,9	0.89	0	5,10,12	1.63	1 (20%)
1	HYP	U	151	1	7,8,9	0.89	0	5,10,12	1.39	1 (20%)
1	KCX	U	201	1,3	7,11,12	0.87	0	7,12,14	1.01	0
1	SMC	U	256	1	5,6,7	0.44	0	2,6,8	1.40	0
1	SMC	U	369	1	5,6,7	0.56	0	2,6,8	1.12	0
1	HYP	V	104	1	7,8,9	0.90	0	5,10,12	1.57	1 (20%)
1	HYP	V	151	1	7,8,9	0.88	0	5,10,12	1.38	1 (20%)
1	KCX	V	201	1,3	7,11,12	0.74	0	7,12,14	0.94	0
1	SMC	V	256	1	5,6,7	0.55	0	2,6,8	1.53	1 (50%)
1	SMC	V	369	1	5,6,7	0.51	0	2,6,8	1.21	0
1	HYP	W	104	1	7,8,9	0.93	0	5,10,12	1.75	1 (20%)
1	HYP	W	151	1	7,8,9	0.91	0	5,10,12	1.41	1 (20%)
1	KCX	W	201	1,3	7,11,12	0.86	0	7,12,14	1.03	0
1	SMC	W	256	1	5,6,7	0.48	0	2,6,8	1.64	0
1	SMC	W	369	1	5,6,7	0.49	0	2,6,8	1.04	0
1	HYP	X	104	1	7,8,9	0.93	0	5,10,12	1.65	1 (20%)
1	HYP	X	151	1	7,8,9	0.90	0	5,10,12	1.35	1 (20%)
1	KCX	X	201	1,3	7,11,12	0.71	0	7,12,14	1.00	0
1	SMC	X	256	1	5,6,7	0.50	0	2,6,8	1.45	0
1	SMC	X	369	1	5,6,7	0.47	0	2,6,8	1.11	0
1	HYP	Y	104	1	7,8,9	0.85	0	5,10,12	1.69	1 (20%)
1	HYP	Y	151	1	7,8,9	0.86	0	5,10,12	1.40	1 (20%)
1	KCX	Y	201	1,3	7,11,12	0.80	0	7,12,14	0.96	0
1	SMC	Y	256	1	5,6,7	0.44	0	2,6,8	1.31	0
1	SMC	Y	369	1	5,6,7	0.68	0	2,6,8	1.08	0
1	HYP	Z	104	1	7,8,9	0.85	0	5,10,12	1.59	1 (20%)
1	HYP	Z	151	1	7,8,9	0.99	0	5,10,12	1.33	1 (20%)
1	KCX	Z	201	1,3	7,11,12	0.81	0	7,12,14	1.01	0
1	SMC	Z	256	1	5,6,7	0.56	0	2,6,8	1.57	0
1	SMC	Z	369	1	5,6,7	0.56	0	2,6,8	1.12	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
2	MME	1	1	2	-	0/4/8/10	0/0/0/0
2	MME	2	1	2	-	0/4/8/10	0/0/0/0
2	MME	3	1	2	-	0/4/8/10	0/0/0/0
2	MME	4	1	2	-	0/4/8/10	0/0/0/0
2	MME	5	1	2	-	0/4/8/10	0/0/0/0
2	MME	6	1	2	-	0/4/8/10	0/0/0/0
2	MME	7	1	2	-	0/4/8/10	0/0/0/0
2	MME	8	1	2	-	0/4/8/10	0/0/0/0
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	A	256	1	-	0/3/5/7	0/0/0/0
1	SMC	A	369	1	-	0/3/5/7	0/0/0/0
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	B	256	1	-	0/3/5/7	0/0/0/0
1	SMC	B	369	1	-	0/3/5/7	0/0/0/0
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	KCX	C	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	C	256	1	-	0/3/5/7	0/0/0/0
1	SMC	C	369	1	-	0/3/5/7	0/0/0/0
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	KCX	D	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	D	256	1	-	0/3/5/7	0/0/0/0
1	SMC	D	369	1	-	0/3/5/7	0/0/0/0
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	E	256	1	-	0/3/5/7	0/0/0/0
1	SMC	E	369	1	-	0/3/5/7	0/0/0/0
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	F	256	1	-	0/3/5/7	0/0/0/0
1	SMC	F	369	1	-	0/3/5/7	0/0/0/0
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	G	256	1	-	0/3/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	G	369	1	-	0/3/5/7	0/0/0/0
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	H	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	H	256	1	-	0/3/5/7	0/0/0/0
1	SMC	H	369	1	-	0/3/5/7	0/0/0/0
2	MME	I	1	2	-	0/4/8/10	0/0/0/0
2	MME	J	1	2	-	0/4/8/10	0/0/0/0
2	MME	K	1	2	-	0/4/8/10	0/0/0/0
2	MME	L	1	2	-	0/4/8/10	0/0/0/0
2	MME	M	1	2	-	0/4/8/10	0/0/0/0
2	MME	N	1	2	-	0/4/8/10	0/0/0/0
2	MME	O	1	2	-	0/4/8/10	0/0/0/0
2	MME	P	1	2	-	0/4/8/10	0/0/0/0
1	HYP	S	104	1	-	0/0/11/13	0/1/1/1
1	HYP	S	151	1	-	0/0/11/13	0/1/1/1
1	KCX	S	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	S	256	1	-	0/3/5/7	0/0/0/0
1	SMC	S	369	1	-	0/3/5/7	0/0/0/0
1	HYP	T	104	1	-	0/0/11/13	0/1/1/1
1	HYP	T	151	1	-	0/0/11/13	0/1/1/1
1	KCX	T	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	T	256	1	-	0/3/5/7	0/0/0/0
1	SMC	T	369	1	-	0/3/5/7	0/0/0/0
1	HYP	U	104	1	-	0/0/11/13	0/1/1/1
1	HYP	U	151	1	-	0/0/11/13	0/1/1/1
1	KCX	U	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	U	256	1	-	0/3/5/7	0/0/0/0
1	SMC	U	369	1	-	0/3/5/7	0/0/0/0
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	V	256	1	-	0/3/5/7	0/0/0/0
1	SMC	V	369	1	-	0/3/5/7	0/0/0/0
1	HYP	W	104	1	-	0/0/11/13	0/1/1/1
1	HYP	W	151	1	-	0/0/11/13	0/1/1/1
1	KCX	W	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	W	256	1	-	0/3/5/7	0/0/0/0
1	SMC	W	369	1	-	0/3/5/7	0/0/0/0
1	HYP	X	104	1	-	0/0/11/13	0/1/1/1
1	HYP	X	151	1	-	0/0/11/13	0/1/1/1
1	KCX	X	201	1,3	-	0/6/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	X	256	1	-	0/3/5/7	0/0/0/0
1	SMC	X	369	1	-	0/3/5/7	0/0/0/0
1	HYP	Y	104	1	-	0/0/11/13	0/1/1/1
1	HYP	Y	151	1	-	0/0/11/13	0/1/1/1
1	KCX	Y	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	Y	256	1	-	0/3/5/7	0/0/0/0
1	SMC	Y	369	1	-	0/3/5/7	0/0/0/0
1	HYP	Z	104	1	-	0/0/11/13	0/1/1/1
1	HYP	Z	151	1	-	0/0/11/13	0/1/1/1
1	KCX	Z	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	Z	256	1	-	0/3/5/7	0/0/0/0
1	SMC	Z	369	1	-	0/3/5/7	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	1	MME	CM-N	-4.84	1.33	1.46
2	J	1	MME	CM-N	-4.82	1.33	1.46
2	6	1	MME	CM-N	-4.80	1.33	1.46
2	P	1	MME	CM-N	-4.79	1.33	1.46
2	3	1	MME	CM-N	-4.79	1.33	1.46

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	104	HYP	O-C-CA	-3.09	117.28	125.44
1	F	104	HYP	O-C-CA	-3.01	117.50	125.44
1	G	104	HYP	O-C-CA	-3.01	117.50	125.44
1	U	104	HYP	O-C-CA	-3.00	117.51	125.44
1	S	104	HYP	O-C-CA	-3.00	117.52	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	3	1	MME	1	0
2	5	1	MME	1	0
2	7	1	MME	2	0
2	8	1	MME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	151	HYP	1	0
1	H	151	HYP	1	0
2	I	1	MME	1	0
2	K	1	MME	1	0
2	L	1	MME	1	0
1	T	151	HYP	1	0
1	U	201	KCX	1	0
1	V	151	HYP	1	0
1	W	151	HYP	1	0
1	X	151	HYP	1	0
1	Y	151	HYP	1	0
1	Z	151	HYP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 16 are monoatomic - leaving 56 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	$\# Z > 2$
4	CAP	A	501	3	14,20,20	1.10	1 (7%)	15,31,31	1.16	2 (13%)
5	GOL	A	605	-	5,5,5	1.02	0	5,5,5	0.38	0
5	GOL	A	613	-	5,5,5	0.95	0	5,5,5	0.33	0
4	CAP	B	501	3	14,20,20	1.10	1 (7%)	15,31,31	1.19	2 (13%)
5	GOL	B	606	-	5,5,5	1.04	0	5,5,5	0.44	0
5	GOL	B	610	-	5,5,5	1.00	0	5,5,5	0.37	0
5	GOL	B	614	-	5,5,5	0.94	0	5,5,5	0.30	0
4	CAP	C	501	3	14,20,20	1.17	1 (7%)	15,31,31	1.18	1 (6%)
5	GOL	C	607	-	5,5,5	0.98	0	5,5,5	0.36	0
5	GOL	C	615	-	5,5,5	0.96	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CAP	D	501	3	14,20,20	1.12	1 (7%)	15,31,31	1.16	2 (13%)
5	GOL	D	608	-	5,5,5	1.02	0	5,5,5	0.28	0
5	GOL	D	616	-	5,5,5	0.99	0	5,5,5	0.47	0
4	CAP	E	501	3	14,20,20	1.07	1 (7%)	15,31,31	1.14	1 (6%)
5	GOL	E	601	-	5,5,5	0.97	0	5,5,5	0.34	0
5	GOL	E	609	-	5,5,5	1.00	0	5,5,5	0.40	0
5	GOL	E	620	-	5,5,5	0.96	0	5,5,5	0.33	0
4	CAP	F	501	3	14,20,20	1.09	1 (7%)	15,31,31	1.17	2 (13%)
5	GOL	F	602	-	5,5,5	0.98	0	5,5,5	0.33	0
5	GOL	F	617	-	5,5,5	0.98	0	5,5,5	0.30	0
4	CAP	G	501	3	14,20,20	1.10	1 (7%)	15,31,31	1.19	2 (13%)
5	GOL	G	603	-	5,5,5	0.99	0	5,5,5	0.32	0
5	GOL	G	611	-	5,5,5	1.04	0	5,5,5	0.39	0
5	GOL	G	618	-	5,5,5	0.94	0	5,5,5	0.34	0
4	CAP	H	501	3	14,20,20	1.07	1 (7%)	15,31,31	1.17	2 (13%)
5	GOL	H	604	-	5,5,5	1.02	0	5,5,5	0.29	0
5	GOL	H	612	-	5,5,5	1.00	0	5,5,5	0.37	0
5	GOL	H	619	-	5,5,5	1.00	0	5,5,5	0.31	0
4	CAP	S	501	3	14,20,20	1.15	1 (7%)	15,31,31	1.16	2 (13%)
5	GOL	S	605	-	5,5,5	0.99	0	5,5,5	0.32	0
5	GOL	S	609	-	5,5,5	0.96	0	5,5,5	0.34	0
5	GOL	S	613	-	5,5,5	0.95	0	5,5,5	0.35	0
4	CAP	T	501	3	14,20,20	1.13	1 (7%)	15,31,31	1.19	2 (13%)
5	GOL	T	606	-	5,5,5	0.99	0	5,5,5	0.34	0
5	GOL	T	614	-	5,5,5	0.99	0	5,5,5	0.33	0
4	CAP	U	501	3	14,20,20	1.17	1 (7%)	15,31,31	1.19	1 (6%)
5	GOL	U	607	-	5,5,5	1.00	0	5,5,5	0.33	0
5	GOL	U	615	-	5,5,5	0.95	0	5,5,5	0.35	0
4	CAP	V	501	3	14,20,20	1.13	1 (7%)	15,31,31	1.18	2 (13%)
5	GOL	V	608	-	5,5,5	1.00	0	5,5,5	0.33	0
5	GOL	V	616	-	5,5,5	0.99	0	5,5,5	0.34	0
4	CAP	W	501	3	14,20,20	1.06	1 (7%)	15,31,31	1.20	2 (13%)
5	GOL	W	601	-	5,5,5	0.98	0	5,5,5	0.35	0
5	GOL	W	620	-	5,5,5	0.97	0	5,5,5	0.45	0
4	CAP	X	501	3	14,20,20	1.08	1 (7%)	15,31,31	1.19	1 (6%)
5	GOL	X	602	-	5,5,5	0.97	0	5,5,5	0.34	0
5	GOL	X	610	-	5,5,5	1.00	0	5,5,5	0.37	0
5	GOL	X	617	-	5,5,5	0.97	0	5,5,5	0.31	0
4	CAP	Y	501	3	14,20,20	1.11	1 (7%)	15,31,31	1.16	1 (6%)
5	GOL	Y	603	-	5,5,5	0.99	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	Y	611	-	5,5,5	1.02	0	5,5,5	0.37	0
5	GOL	Y	618	-	5,5,5	0.99	0	5,5,5	0.34	0
4	CAP	Z	501	3	14,20,20	1.09	1 (7%)	15,31,31	1.19	2 (13%)
5	GOL	Z	604	-	5,5,5	0.97	0	5,5,5	0.34	0
5	GOL	Z	612	-	5,5,5	1.01	0	5,5,5	0.36	0
5	GOL	Z	619	-	5,5,5	0.96	0	5,5,5	0.34	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
4	CAP	A	501	3	-	0/23/29/29	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
5	GOL	A	613	-	-	0/4/4/4	0/0/0/0
4	CAP	B	501	3	-	0/23/29/29	0/0/0/0
5	GOL	B	606	-	-	0/4/4/4	0/0/0/0
5	GOL	B	610	-	-	0/4/4/4	0/0/0/0
5	GOL	B	614	-	-	0/4/4/4	0/0/0/0
4	CAP	C	501	3	-	0/23/29/29	0/0/0/0
5	GOL	C	607	-	-	0/4/4/4	0/0/0/0
5	GOL	C	615	-	-	0/4/4/4	0/0/0/0
4	CAP	D	501	3	-	0/23/29/29	0/0/0/0
5	GOL	D	608	-	-	0/4/4/4	0/0/0/0
5	GOL	D	616	-	-	0/4/4/4	0/0/0/0
4	CAP	E	501	3	-	0/23/29/29	0/0/0/0
5	GOL	E	601	-	-	0/4/4/4	0/0/0/0
5	GOL	E	609	-	-	0/4/4/4	0/0/0/0
5	GOL	E	620	-	-	0/4/4/4	0/0/0/0
4	CAP	F	501	3	-	0/23/29/29	0/0/0/0
5	GOL	F	602	-	-	0/4/4/4	0/0/0/0
5	GOL	F	617	-	-	0/4/4/4	0/0/0/0
4	CAP	G	501	3	-	0/23/29/29	0/0/0/0
5	GOL	G	603	-	-	0/4/4/4	0/0/0/0
5	GOL	G	611	-	-	0/4/4/4	0/0/0/0
5	GOL	G	618	-	-	0/4/4/4	0/0/0/0
4	CAP	H	501	3	-	0/23/29/29	0/0/0/0
5	GOL	H	604	-	-	0/4/4/4	0/0/0/0
5	GOL	H	612	-	-	0/4/4/4	0/0/0/0
5	GOL	H	619	-	-	0/4/4/4	0/0/0/0
4	CAP	S	501	3	-	0/23/29/29	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	S	605	-	-	0/4/4/4	0/0/0/0
5	GOL	S	609	-	-	0/4/4/4	0/0/0/0
5	GOL	S	613	-	-	0/4/4/4	0/0/0/0
4	CAP	T	501	3	-	0/23/29/29	0/0/0/0
5	GOL	T	606	-	-	0/4/4/4	0/0/0/0
5	GOL	T	614	-	-	0/4/4/4	0/0/0/0
4	CAP	U	501	3	-	0/23/29/29	0/0/0/0
5	GOL	U	607	-	-	0/4/4/4	0/0/0/0
5	GOL	U	615	-	-	0/4/4/4	0/0/0/0
4	CAP	V	501	3	-	0/23/29/29	0/0/0/0
5	GOL	V	608	-	-	0/4/4/4	0/0/0/0
5	GOL	V	616	-	-	0/4/4/4	0/0/0/0
4	CAP	W	501	3	-	0/23/29/29	0/0/0/0
5	GOL	W	601	-	-	0/4/4/4	0/0/0/0
5	GOL	W	620	-	-	0/4/4/4	0/0/0/0
4	CAP	X	501	3	-	0/23/29/29	0/0/0/0
5	GOL	X	602	-	-	0/4/4/4	0/0/0/0
5	GOL	X	610	-	-	0/4/4/4	0/0/0/0
5	GOL	X	617	-	-	0/4/4/4	0/0/0/0
4	CAP	Y	501	3	-	0/23/29/29	0/0/0/0
5	GOL	Y	603	-	-	0/4/4/4	0/0/0/0
5	GOL	Y	611	-	-	0/4/4/4	0/0/0/0
5	GOL	Y	618	-	-	0/4/4/4	0/0/0/0
4	CAP	Z	501	3	-	0/23/29/29	0/0/0/0
5	GOL	Z	604	-	-	0/4/4/4	0/0/0/0
5	GOL	Z	612	-	-	0/4/4/4	0/0/0/0
5	GOL	Z	619	-	-	0/4/4/4	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	501	CAP	C5-C4	2.29	1.55	1.51
4	X	501	CAP	C5-C4	2.29	1.55	1.51
4	W	501	CAP	C5-C4	2.37	1.55	1.51
4	F	501	CAP	C5-C4	2.42	1.55	1.51
4	E	501	CAP	C5-C4	2.44	1.55	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	501	CAP	O5P-P2-O4P	2.01	117.06	110.58
4	A	501	CAP	O5P-P2-O4P	2.02	117.07	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	CAP	O5P-P2-O4P	2.03	117.11	110.58
4	H	501	CAP	O5P-P2-O4P	2.06	117.21	110.58
4	V	501	CAP	O5P-P2-O4P	2.07	117.23	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	GOL	1	0
5	B	606	GOL	2	0
5	C	615	GOL	1	0
5	D	616	GOL	1	0
5	F	617	GOL	1	0
5	H	619	GOL	1	0
5	V	616	GOL	1	0
5	W	620	GOL	1	0
5	Y	618	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/475 (97%)	-0.34	6 (1%) 79 78	5, 12, 27, 61	0
1	B	462/475 (97%)	-0.41	5 (1%) 82 81	7, 13, 28, 43	0
1	C	461/475 (97%)	-0.49	3 (0%) 89 88	6, 11, 24, 49	0
1	D	462/475 (97%)	-0.49	5 (1%) 82 81	6, 10, 23, 46	0
1	E	460/475 (96%)	-0.51	3 (0%) 89 88	6, 11, 24, 40	0
1	F	460/475 (96%)	-0.47	2 (0%) 93 92	7, 12, 24, 43	0
1	G	461/475 (97%)	-0.47	4 (0%) 85 85	6, 10, 24, 39	0
1	H	463/475 (97%)	-0.56	4 (0%) 85 85	4, 10, 22, 57	0
1	S	460/475 (96%)	-0.42	2 (0%) 93 92	6, 12, 27, 49	0
1	T	461/475 (97%)	-0.40	4 (0%) 85 85	6, 12, 27, 48	0
1	U	464/475 (97%)	-0.42	7 (1%) 76 74	6, 12, 27, 62	0
1	V	464/475 (97%)	-0.37	8 (1%) 73 71	5, 11, 26, 66	0
1	W	461/475 (97%)	-0.39	5 (1%) 82 81	6, 13, 29, 43	0
1	X	461/475 (97%)	-0.34	6 (1%) 79 78	6, 12, 27, 48	0
1	Y	460/475 (96%)	-0.43	5 (1%) 82 81	6, 11, 27, 45	0
1	Z	461/475 (97%)	-0.53	3 (0%) 89 88	5, 10, 23, 54	0
2	1	139/140 (99%)	-0.18	3 (2%) 65 62	8, 17, 30, 39	0
2	2	139/140 (99%)	-0.22	2 (1%) 78 76	9, 18, 31, 43	0
2	3	139/140 (99%)	-0.14	1 (0%) 89 88	9, 19, 34, 44	0
2	4	139/140 (99%)	-0.25	1 (0%) 89 88	9, 16, 30, 37	0
2	5	139/140 (99%)	-0.33	0 100 100	9, 16, 29, 38	0
2	6	139/140 (99%)	-0.20	0 100 100	9, 19, 33, 40	0
2	7	139/140 (99%)	-0.33	2 (1%) 78 76	8, 15, 28, 34	0
2	8	139/140 (99%)	-0.45	0 100 100	7, 14, 28, 34	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	I	139/140 (99%)	-0.18	3 (2%) 65 62	10, 18, 34, 45	0
2	J	139/140 (99%)	-0.15	3 (2%) 65 62	10, 20, 34, 42	0
2	K	139/140 (99%)	-0.23	1 (0%) 89 88	8, 17, 31, 39	0
2	L	139/140 (99%)	-0.31	1 (0%) 89 88	9, 16, 30, 39	0
2	M	139/140 (99%)	-0.31	2 (1%) 78 76	8, 15, 31, 39	0
2	N	139/140 (99%)	-0.26	2 (1%) 78 76	8, 17, 29, 39	0
2	O	139/140 (99%)	-0.36	0 100 100	8, 14, 28, 36	0
2	P	139/140 (99%)	-0.37	2 (1%) 78 76	8, 14, 27, 37	0
All	All	9608/9840 (97%)	-0.40	95 (0%) 84 83	4, 12, 28, 66	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	10	GLY	8.7
1	T	10	GLY	8.5
1	D	9	ALA	8.1
1	X	10	GLY	7.4
1	V	7	THR	7.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	HYP	S	104	8/9	0.97	0.07	-	11,12,13,14	0
1	SMC	S	369	7/8	0.99	0.04	-	10,10,12,12	0
1	SMC	Y	256	7/8	0.99	0.05	-	6,7,8,8	0
1	SMC	F	256	7/8	0.99	0.05	-	8,9,9,9	0
1	SMC	D	256	7/8	0.99	0.05	-	5,7,8,10	0
1	HYP	Z	151	8/9	0.98	0.06	-	6,7,8,9	0
2	MME	J	1	9/10	0.94	0.12	-	20,23,31,31	0
1	SMC	G	256	7/8	0.99	0.06	-	5,6,8,8	0
1	SMC	B	256	7/8	0.99	0.05	-	7,8,9,9	0
1	SMC	W	256	7/8	0.99	0.05	-	8,9,9,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SMC	X	369	7/8	0.98	0.05	-	11,12,13,14	0
1	KCX	Z	201	12/13	0.97	0.10	-	4,7,8,9	0
1	SMC	E	256	7/8	0.99	0.05	-	6,7,8,8	0
1	SMC	G	369	7/8	0.99	0.06	-	11,11,13,13	0
1	HYP	H	151	8/9	0.98	0.07	-	5,5,6,6	0
1	SMC	B	369	7/8	0.98	0.06	-	12,13,13,14	0
1	SMC	A	256	7/8	0.99	0.05	-	7,8,8,8	0
1	HYP	X	104	8/9	0.97	0.07	-	10,10,11,11	0
2	MME	4	1	9/10	0.93	0.12	-	24,25,30,30	0
1	HYP	T	104	8/9	0.95	0.07	-	9,11,12,14	0
1	KCX	F	201	12/13	0.96	0.11	-	5,8,10,10	0
1	HYP	A	151	8/9	0.97	0.07	-	8,8,9,11	0
1	HYP	T	151	8/9	0.97	0.07	-	6,7,8,9	0
1	HYP	X	151	8/9	0.97	0.07	-	7,9,10,10	0
1	KCX	T	201	12/13	0.98	0.08	-	4,8,9,9	0
1	HYP	S	151	8/9	0.98	0.07	-	7,8,9,9	0
1	HYP	Y	104	8/9	0.98	0.06	-	10,11,11,12	0
2	MME	L	1	9/10	0.93	0.13	-	18,24,30,30	0
1	HYP	C	151	8/9	0.98	0.07	-	7,8,9,9	0
1	HYP	H	104	8/9	0.98	0.05	-	6,7,8,9	0
2	MME	5	1	9/10	0.95	0.09	-	18,21,30,31	0
2	MME	3	1	9/10	0.93	0.14	-	24,26,34,34	0
2	MME	P	1	9/10	0.97	0.10	-	17,21,25,25	0
1	KCX	C	201	12/13	0.97	0.10	-	7,9,11,11	0
2	MME	1	1	9/10	0.95	0.11	-	21,23,24,25	0
1	SMC	T	256	7/8	0.99	0.05	-	6,6,7,8	0
1	SMC	Y	369	7/8	0.98	0.05	-	11,12,13,14	0
1	HYP	Y	151	8/9	0.98	0.06	-	8,9,9,9	0
1	SMC	U	369	7/8	0.99	0.05	-	8,9,10,11	0
1	HYP	G	151	8/9	0.97	0.06	-	9,9,10,11	0
1	KCX	S	201	12/13	0.97	0.12	-	5,8,8,11	0
1	HYP	B	151	8/9	0.98	0.07	-	9,10,11,12	0
1	SMC	C	256	7/8	0.99	0.05	-	7,8,9,10	0
2	MME	N	1	9/10	0.92	0.12	-	18,20,28,31	0
1	HYP	D	151	8/9	0.98	0.07	-	4,7,8,8	0
1	HYP	V	104	8/9	0.97	0.07	-	8,9,10,10	0
1	HYP	W	104	8/9	0.97	0.07	-	10,11,11,12	0
1	KCX	X	201	12/13	0.97	0.10	-	7,8,10,10	0
1	KCX	W	201	12/13	0.97	0.10	-	9,10,12,12	0
2	MME	2	1	9/10	0.96	0.09	-	21,23,27,27	0
2	MME	7	1	9/10	0.96	0.11	-	16,18,27,29	0
1	KCX	G	201	12/13	0.97	0.13	-	5,7,8,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	KCX	D	201	12/13	0.98	0.10	-	6,7,7,8	0
1	HYP	V	151	8/9	0.98	0.06	-	7,7,9,9	0
1	KCX	E	201	12/13	0.97	0.08	-	6,8,10,11	0
1	KCX	V	201	12/13	0.96	0.14	-	8,9,11,11	0
1	KCX	H	201	12/13	0.97	0.10	-	5,6,7,9	0
2	MME	8	1	9/10	0.94	0.14	-	21,24,27,30	0
1	KCX	B	201	12/13	0.97	0.10	-	7,10,11,12	0
1	HYP	E	104	8/9	0.96	0.07	-	7,9,10,10	0
1	SMC	C	369	7/8	0.99	0.05	-	8,10,12,12	0
1	SMC	V	256	7/8	0.99	0.04	-	6,6,7,8	0
1	HYP	A	104	8/9	0.97	0.08	-	10,11,12,14	0
1	HYP	B	104	8/9	0.97	0.06	-	8,11,11,13	0
1	SMC	E	369	7/8	0.99	0.04	-	8,9,10,11	0
2	MME	O	1	9/10	0.95	0.12	-	18,21,28,31	0
1	SMC	F	369	7/8	0.99	0.04	-	10,11,12,13	0
1	SMC	Z	369	7/8	0.99	0.05	-	8,9,11,12	0
1	HYP	C	104	8/9	0.98	0.06	-	6,8,9,9	0
1	SMC	H	256	7/8	0.99	0.05	-	6,6,7,8	0
2	MME	K	1	9/10	0.94	0.12	-	22,24,28,29	0
1	HYP	Z	104	8/9	0.98	0.06	-	8,9,10,12	0
1	KCX	Y	201	12/13	0.97	0.10	-	6,7,8,8	0
1	HYP	U	104	8/9	0.97	0.06	-	9,9,9,9	0
1	SMC	S	256	7/8	0.99	0.05	-	4,6,7,7	0
1	SMC	W	369	7/8	0.98	0.07	-	9,10,11,11	0
1	HYP	W	151	8/9	0.98	0.07	-	5,8,9,9	0
1	SMC	H	369	7/8	0.99	0.04	-	6,9,10,10	0
1	SMC	D	369	7/8	0.99	0.05	-	8,9,10,10	0
2	MME	6	1	9/10	0.96	0.10	-	20,21,26,27	0
1	SMC	V	369	7/8	0.99	0.05	-	10,10,12,14	0
2	MME	I	1	9/10	0.96	0.09	-	20,21,28,28	0
1	SMC	T	369	7/8	0.99	0.05	-	11,12,13,15	0
1	HYP	U	151	8/9	0.98	0.07	-	7,9,9,9	0
1	SMC	Z	256	7/8	0.99	0.04	-	6,7,7,8	0
1	SMC	X	256	7/8	0.99	0.05	-	7,7,9,11	0
1	KCX	U	201	12/13	0.98	0.12	-	8,10,11,11	0
1	SMC	U	256	7/8	0.99	0.05	-	5,7,7,7	0
1	HYP	E	151	8/9	0.97	0.08	-	8,9,10,10	0
1	HYP	D	104	8/9	0.97	0.07	-	6,7,9,9	0
1	HYP	F	151	8/9	0.97	0.08	-	11,11,12,12	0
2	MME	M	1	9/10	0.94	0.13	-	21,22,30,31	0
1	HYP	F	104	8/9	0.98	0.05	-	8,10,12,14	0
1	HYP	G	104	8/9	0.98	0.06	-	9,11,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SMC	A	369	7/8	0.98	0.06	-	13,13,15,16	0
1	KCX	A	201	12/13	0.96	0.14	-	7,9,10,11	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	C	615	6/6	0.85	0.15	13.91	26,28,31,32	0
5	GOL	Y	618	6/6	0.80	0.19	13.04	37,40,41,41	0
5	GOL	W	620	6/6	0.90	0.14	12.42	34,36,36,37	0
5	GOL	D	616	6/6	0.86	0.17	12.19	22,26,30,32	0
5	GOL	H	619	6/6	0.80	0.17	10.87	29,32,34,34	0
5	GOL	V	616	6/6	0.90	0.14	9.50	25,27,29,30	0
5	GOL	B	614	6/6	0.90	0.15	9.42	25,31,33,34	0
5	GOL	H	604	6/6	0.70	0.20	8.46	25,30,33,34	0
5	GOL	F	617	6/6	0.84	0.18	7.41	32,32,33,34	0
5	GOL	S	609	6/6	0.90	0.18	5.84	23,25,28,32	0
5	GOL	E	620	6/6	0.90	0.14	5.48	22,26,28,28	0
5	GOL	H	612	6/6	0.89	0.15	5.24	14,18,21,21	0
5	GOL	X	617	6/6	0.91	0.11	5.23	21,27,29,30	0
5	GOL	S	613	6/6	0.92	0.12	5.20	23,25,25,26	0
5	GOL	G	611	6/6	0.87	0.17	4.36	16,18,23,26	0
5	GOL	E	609	6/6	0.90	0.14	4.22	14,17,20,22	0
5	GOL	Z	612	6/6	0.89	0.17	4.21	17,19,22,23	0
5	GOL	Y	611	6/6	0.92	0.15	3.63	19,21,22,23	0
5	GOL	G	618	6/6	0.93	0.09	3.40	26,30,31,31	0
5	GOL	E	601	6/6	0.93	0.12	3.32	29,30,30,31	0
5	GOL	V	608	6/6	0.91	0.13	2.79	17,19,20,21	0
5	GOL	D	608	6/6	0.89	0.13	2.75	23,26,27,27	0
5	GOL	X	610	6/6	0.93	0.15	2.73	16,19,22,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	Z	619	6/6	0.93	0.09	2.62	19,24,25,26	0
5	GOL	A	605	6/6	0.90	0.13	2.60	26,27,29,30	0
5	GOL	B	606	6/6	0.90	0.13	2.35	22,22,24,24	0
5	GOL	A	613	6/6	0.94	0.09	2.29	25,29,30,30	0
5	GOL	U	607	6/6	0.89	0.12	2.26	23,27,28,28	0
5	GOL	Z	604	6/6	0.92	0.12	2.23	24,26,26,28	0
5	GOL	T	614	6/6	0.94	0.08	1.93	22,27,29,29	0
5	GOL	B	610	6/6	0.95	0.13	1.76	18,20,21,23	0
5	GOL	Y	603	6/6	0.90	0.12	1.64	29,31,32,32	0
5	GOL	W	601	6/6	0.93	0.12	1.64	23,25,25,25	0
5	GOL	X	602	6/6	0.96	0.09	1.49	19,20,22,22	0
5	GOL	G	603	6/6	0.93	0.11	1.16	20,22,25,27	0
5	GOL	U	615	6/6	0.95	0.08	1.05	20,23,25,27	0
5	GOL	C	607	6/6	0.94	0.09	1.00	23,24,26,27	0
5	GOL	T	606	6/6	0.92	0.12	0.98	21,22,24,25	0
3	MG	G	476	1/1	0.99	0.11	0.87	11,11,11,11	0
5	GOL	S	605	6/6	0.91	0.10	0.83	26,28,30,30	0
3	MG	X	476	1/1	0.99	0.11	0.80	13,13,13,13	0
3	MG	C	476	1/1	1.00	0.10	0.74	13,13,13,13	0
3	MG	E	476	1/1	0.99	0.08	0.59	11,11,11,11	0
3	MG	Z	476	1/1	1.00	0.09	0.48	9,9,9,9	0
4	CAP	S	501	21/21	0.98	0.10	0.36	10,12,12,13	0
3	MG	A	476	1/1	0.99	0.12	0.27	9,9,9,9	0
3	MG	V	476	1/1	0.99	0.10	0.25	12,12,12,12	0
3	MG	H	476	1/1	0.98	0.10	0.21	10,10,10,10	0
3	MG	B	476	1/1	1.00	0.08	0.20	11,11,11,11	0
3	MG	W	476	1/1	0.99	0.09	0.08	12,12,12,12	0
3	MG	S	476	1/1	0.99	0.11	0.08	11,11,11,11	0
4	CAP	C	501	21/21	0.98	0.09	0.01	8,10,11,13	0
3	MG	D	476	1/1	1.00	0.08	-0.30	9,9,9,9	0
4	CAP	A	501	21/21	0.98	0.10	-0.31	7,10,11,14	0
4	CAP	X	501	21/21	0.98	0.10	-0.34	8,11,13,14	0
4	CAP	Z	501	21/21	0.98	0.07	-0.40	7,9,10,11	0
4	CAP	V	501	21/21	0.98	0.09	-0.43	8,10,11,12	0
4	CAP	F	501	21/21	0.98	0.08	-0.46	9,11,13,15	0
4	CAP	U	501	21/21	0.98	0.09	-0.49	11,13,14,16	0
4	CAP	G	501	21/21	0.99	0.08	-0.57	6,8,10,11	0
4	CAP	W	501	21/21	0.98	0.08	-0.60	9,11,15,17	0
5	GOL	F	602	6/6	0.94	0.07	-0.61	22,24,25,27	0
4	CAP	T	501	21/21	0.98	0.07	-0.71	6,10,11,12	0
4	CAP	H	501	21/21	0.99	0.08	-0.71	6,8,9,11	0
3	MG	U	476	1/1	0.98	0.09	-0.74	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CAP	D	501	21/21	0.99	0.07	-0.79	6,9,10,12	0
4	CAP	Y	501	21/21	0.98	0.08	-0.82	6,8,10,11	0
4	CAP	B	501	21/21	0.98	0.07	-0.82	10,12,15,17	0
3	MG	Y	476	1/1	0.99	0.08	-0.84	11,11,11,11	0
4	CAP	E	501	21/21	0.98	0.07	-0.86	8,11,11,12	0
3	MG	T	476	1/1	0.99	0.05	-1.97	12,12,12,12	0
3	MG	F	476	1/1	0.99	0.06	-3.69	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.