



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:41 am GMT

PDB ID : 3AXM  
Title : Structure of rice Rubisco in complex with 6PG  
Authors : Matsumura, H.; Mizohata, E.; Ishida, H.; Kogami, A.; Ueno, T.; Makino, A.;  
Inoue, T.; Yokota, A.; Mae, T.; Kai, Y.  
Deposited on : 2011-04-11  
Resolution : 1.65 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

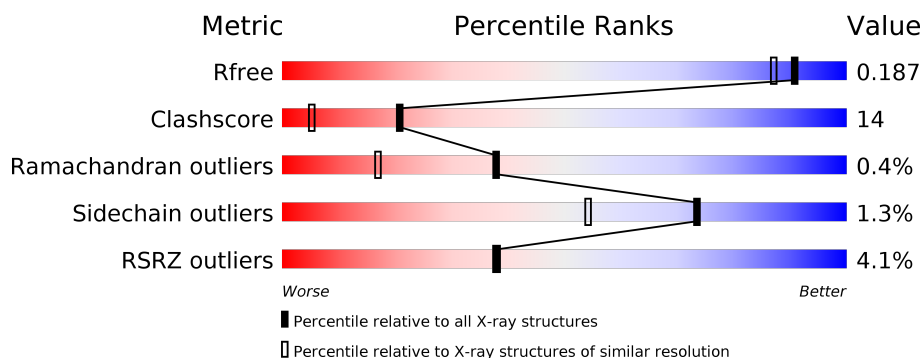
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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.



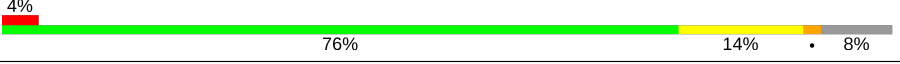

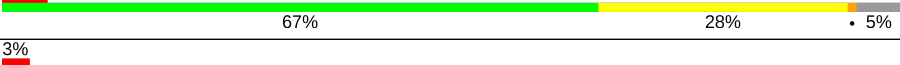

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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  $\geq 3$ , 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	477	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>7%</div> </div> </div>
1	B	477	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>7%</div> </div> </div>
1	C	477	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>7%</div> </div> </div>
1	D	477	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
1	E	477	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</div> </div> </div>
1	F	477	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	477	
1	H	477	
2	S	129	
2	T	129	
2	U	129	
2	V	129	
2	W	129	
2	X	129	
2	Y	129	
2	Z	129	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39557 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3464	2193	614	637	20			
1	B	443	Total	C	N	O	S	0	0	0
			3461	2192	613	636	20			
1	C	443	Total	C	N	O	S	0	0	0
			3459	2191	612	636	20			
1	D	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			
1	E	441	Total	C	N	O	S	0	0	0
			3445	2181	610	634	20			
1	F	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			
1	G	441	Total	C	N	O	S	0	0	0
			3445	2181	610	634	20			
1	H	444	Total	C	N	O	S	0	0	0
			3468	2197	614	637	20			

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	T	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	U	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	V	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	W	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	X	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			
2	Z	123	Total	C	N	O	S	0	0	1
			1016	672	163	175	6			

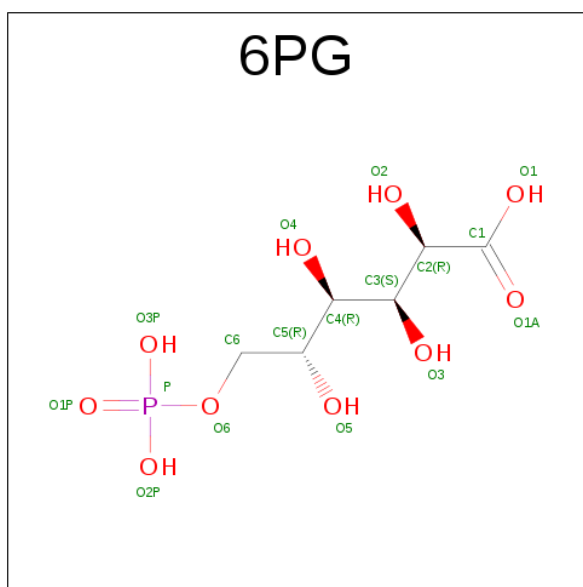
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	NME	-	AMIDATION	UNP Q0INY7
T	0	NME	-	AMIDATION	UNP Q0INY7
U	0	NME	-	AMIDATION	UNP Q0INY7
V	0	NME	-	AMIDATION	UNP Q0INY7
W	0	NME	-	AMIDATION	UNP Q0INY7
X	0	NME	-	AMIDATION	UNP Q0INY7
Y	0	NME	-	AMIDATION	UNP Q0INY7
Z	0	NME	-	AMIDATION	UNP Q0INY7

- 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		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SUGAR (6-PHOSPHOGLUCONIC ACID) (three-letter code: 6PG) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			17	6	10	1		
4	B	1	Total	C	O	P	0	0
			17	6	10	1		
4	C	1	Total	C	O	P	0	0
			17	6	10	1		
4	D	1	Total	C	O	P	0	0
			17	6	10	1		
4	E	1	Total	C	O	P	0	0
			17	6	10	1		
4	F	1	Total	C	O	P	0	0
			17	6	10	1		
4	G	1	Total	C	O	P	0	0
			17	6	10	1		
4	H	1	Total	C	O	P	0	0
			17	6	10	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	309	Total	O	0	0
			309	309		
5	S	113	Total	O	0	0
			113	113		
5	B	345	Total	O	0	0
			345	345		
5	T	99	Total	O	0	0
			99	99		

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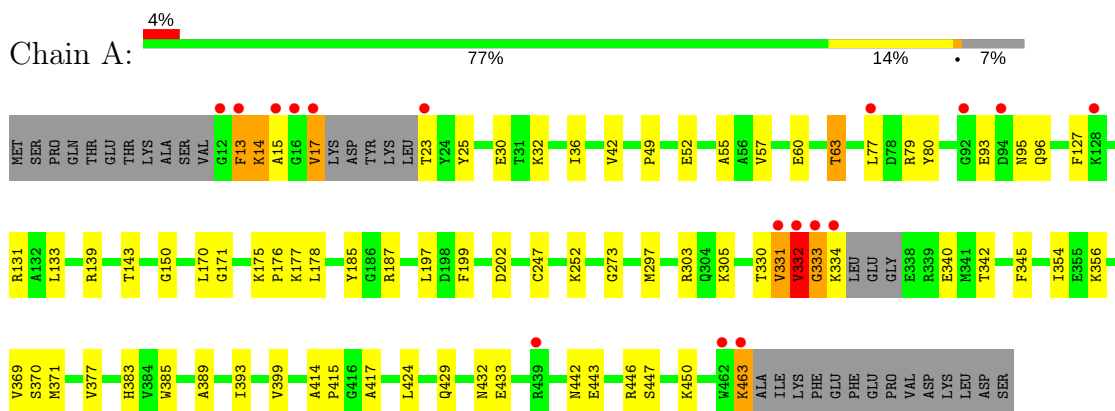
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	339	Total 339	O 339	0	0
5	U	125	Total 125	O 125	0	0
5	D	335	Total 335	O 335	0	0
5	V	123	Total 123	O 123	0	0
5	E	318	Total 318	O 318	0	0
5	W	122	Total 122	O 122	0	0
5	F	371	Total 371	O 371	0	0
5	X	115	Total 115	O 115	0	0
5	G	341	Total 341	O 341	0	0
5	Y	111	Total 111	O 111	0	0
5	H	326	Total 326	O 326	0	0
5	Z	115	Total 115	O 115	0	0

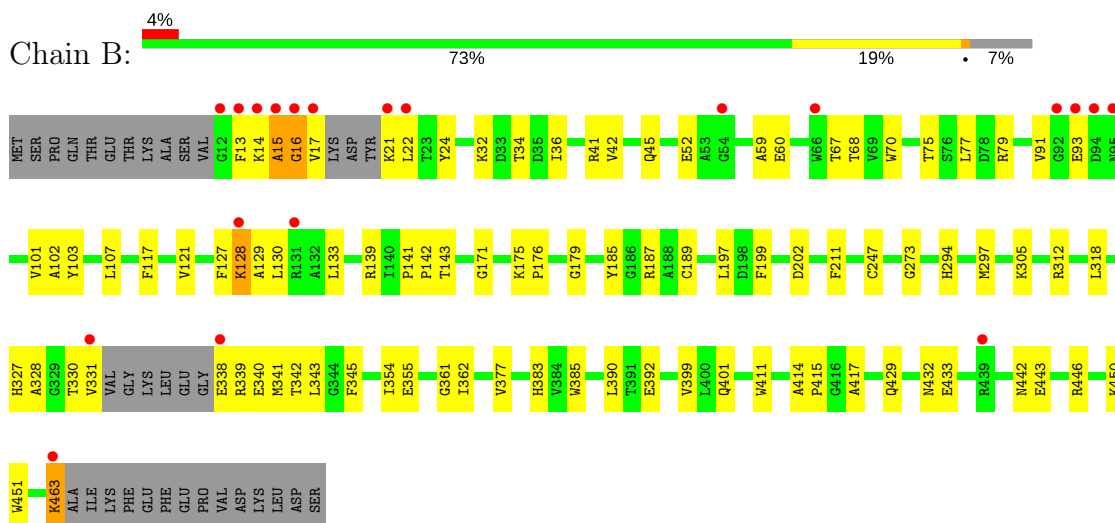
### 3 Residue-property plots [i](#)

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.

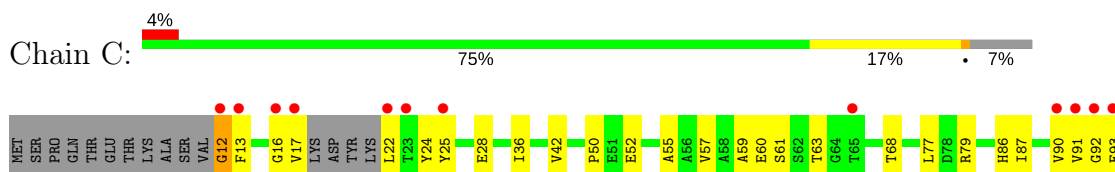
#### • Molecule 1: Ribulose biphosphate carboxylase large chain



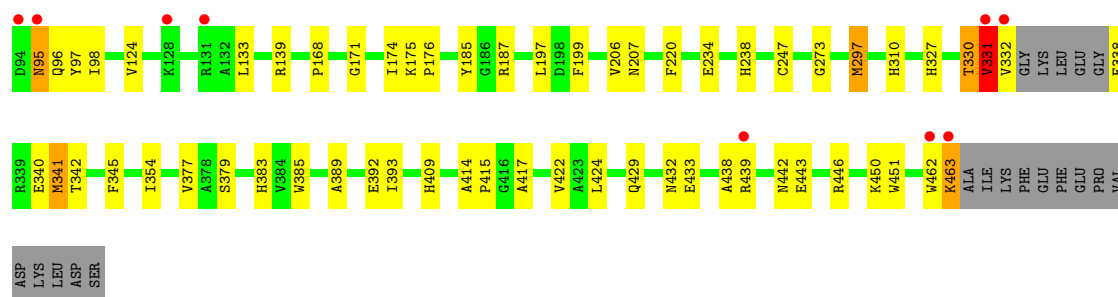
#### • Molecule 1: Ribulose biphosphate carboxylase large chain



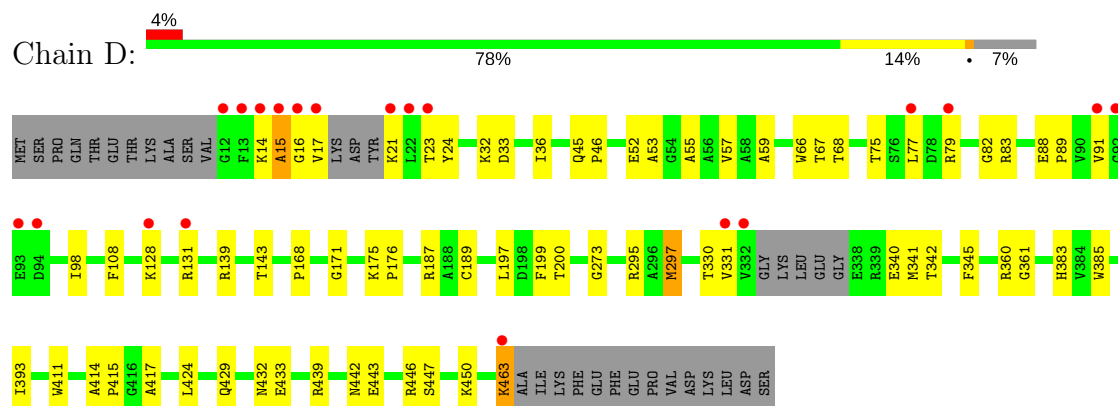
#### • Molecule 1: Ribulose biphosphate carboxylase large chain



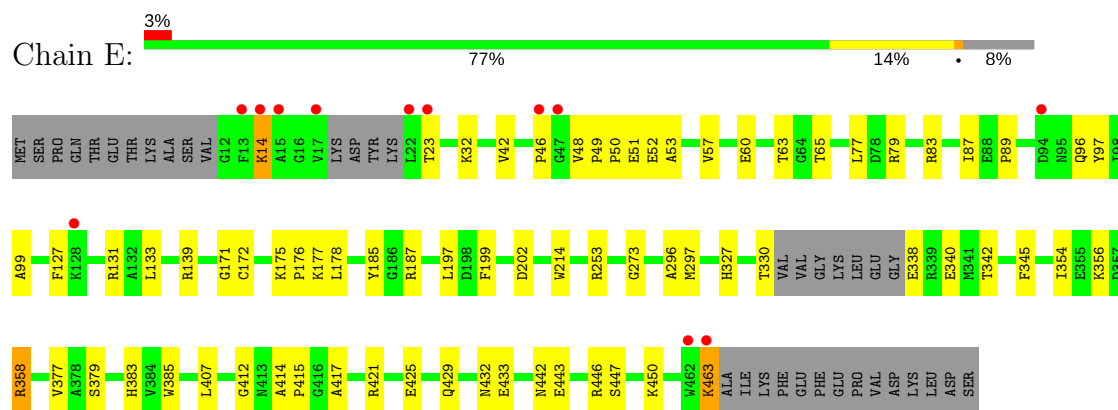




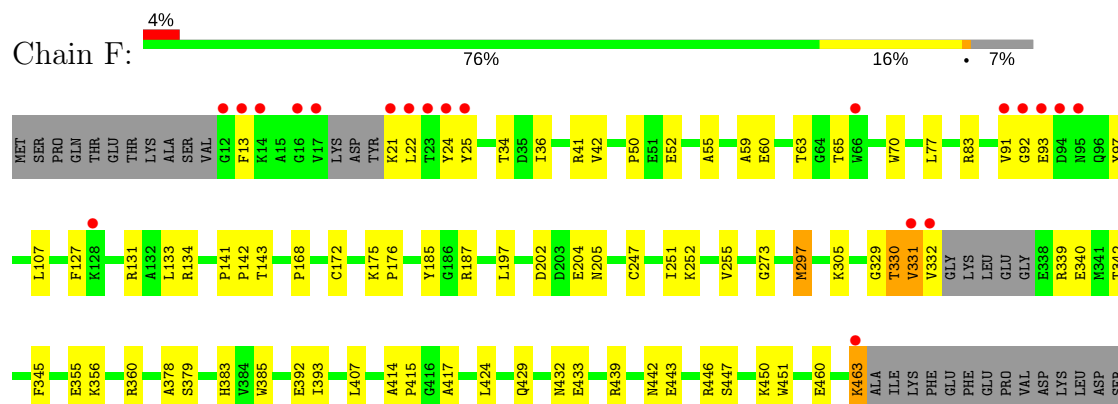
- Molecule 1: Ribulose biphosphate carboxylase large chain



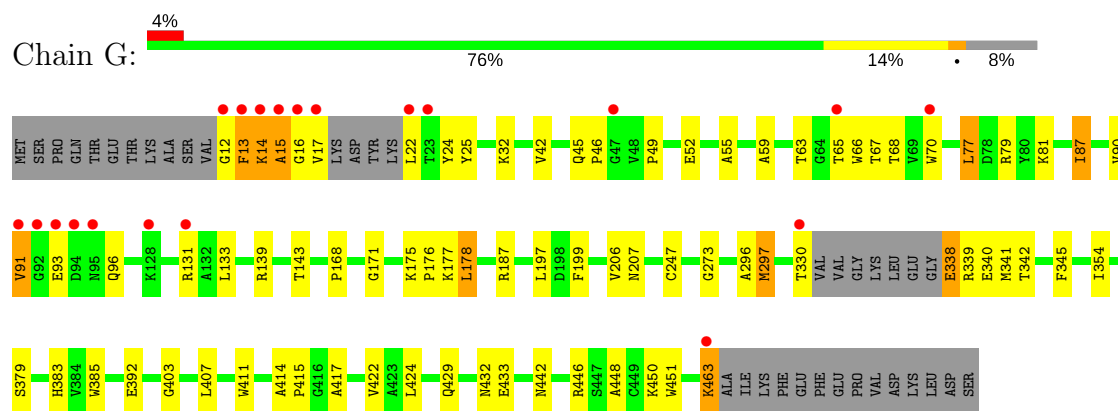
- Molecule 1: Ribulose biphosphate carboxylase large chain



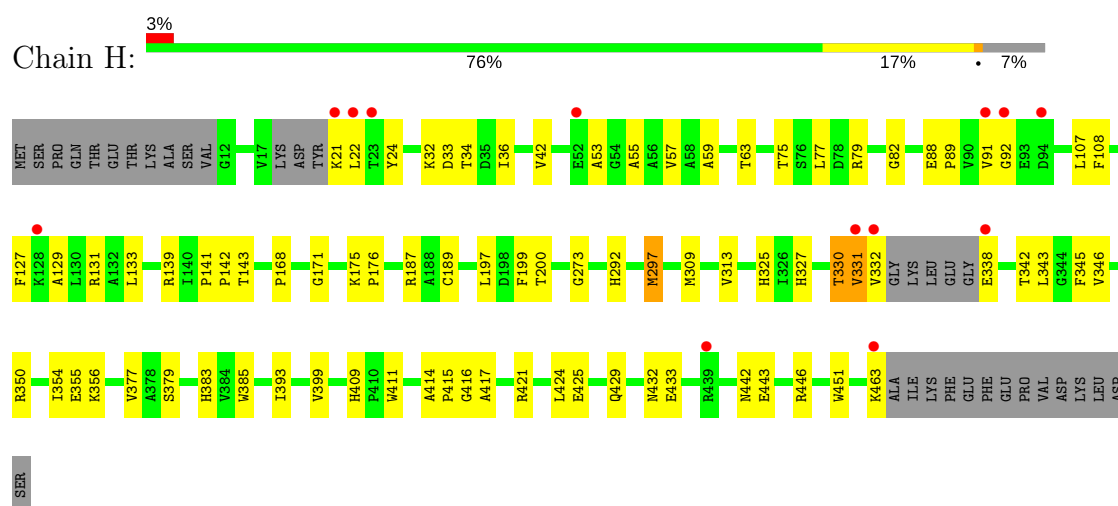
- Molecule 1: Ribulose biphosphate carboxylase large chain



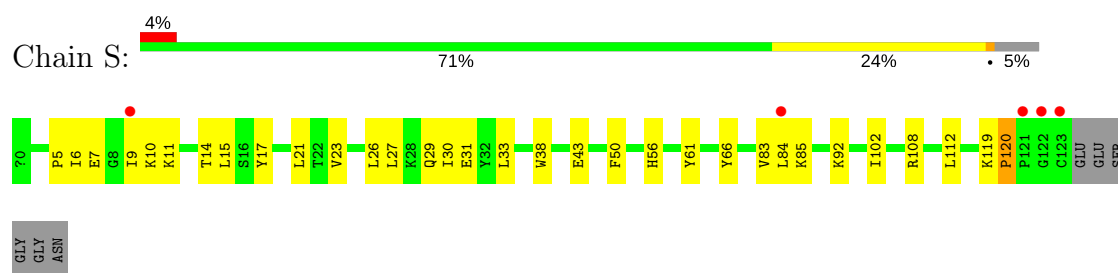
- Molecule 1: Ribulose biphosphate carboxylase large chain



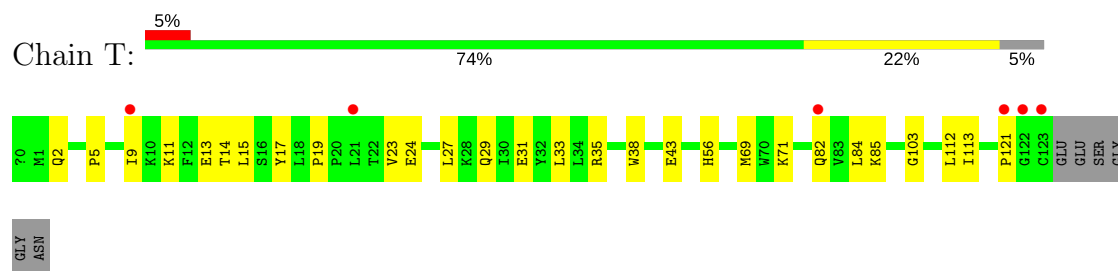
- Molecule 1: Ribulose biphosphate carboxylase large chain



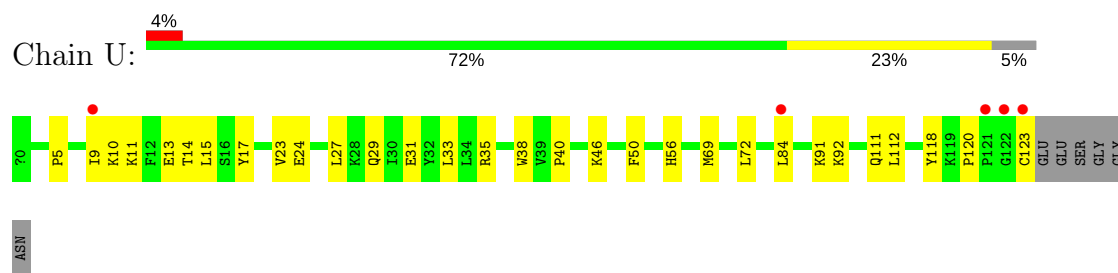
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



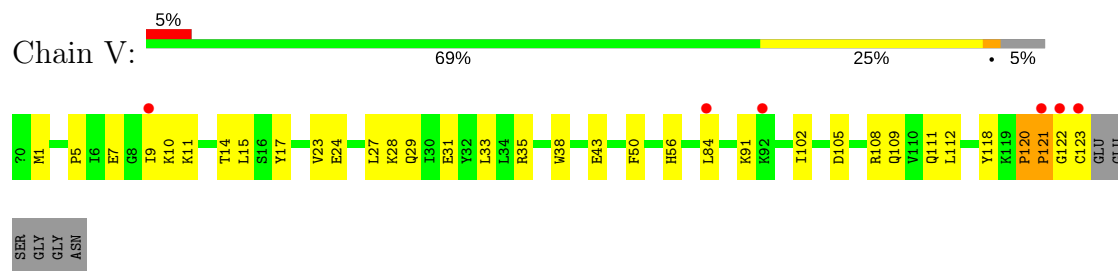
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



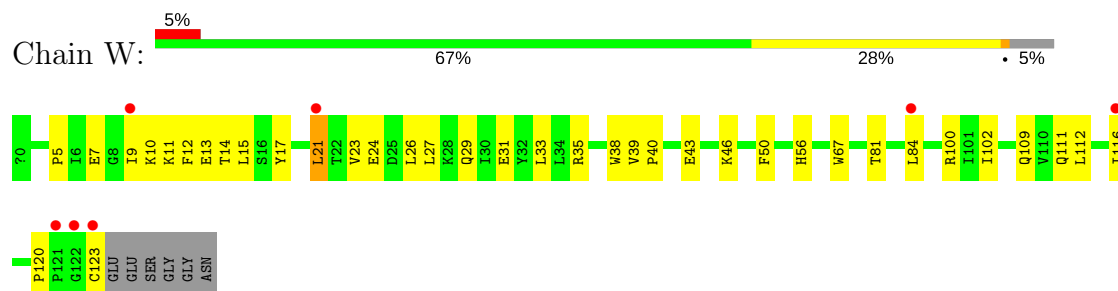
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



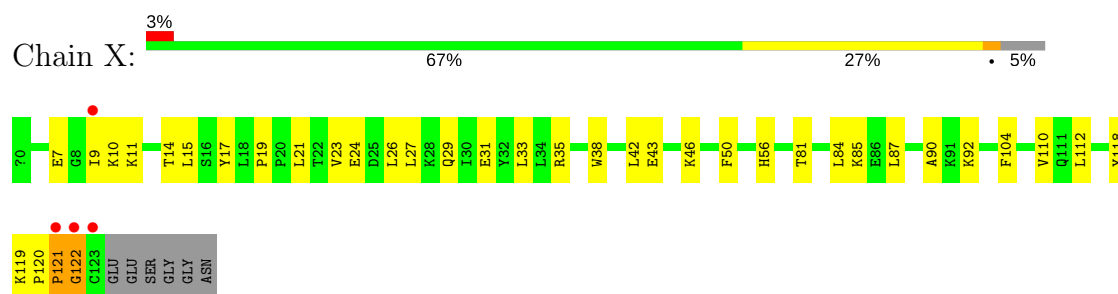
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



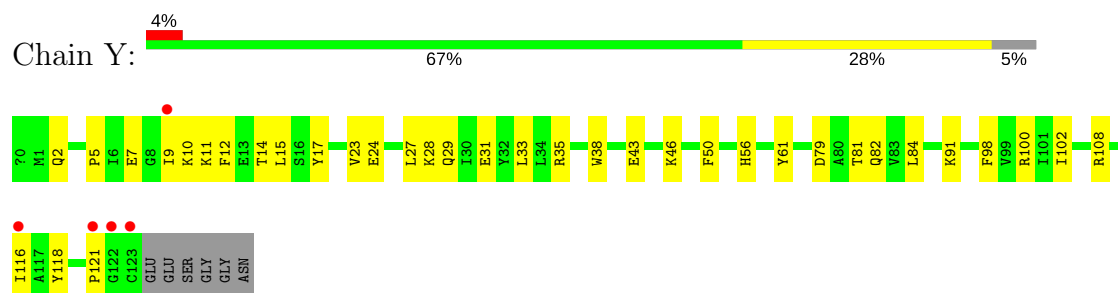
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



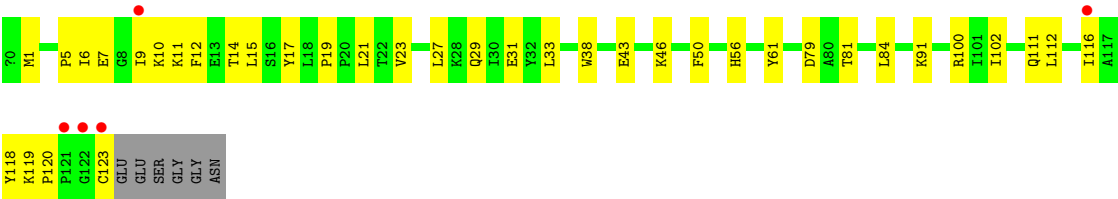
- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



● Molecule 2: Ribulose biphosphate carboxylase small chain, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.41Å 199.62Å 111.17Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	74.26 – 1.65 74.26 – 1.55	Depositor EDS
% Data completeness (in resolution range)	85.2 (74.26-1.65) 83.5 (74.26-1.55)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.55Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.190 0.169 , 0.187	Depositor DCC
$R_{free}$ test set	24291 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.3	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for l,k,-h 0.028 for h,-k,-l 0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	39557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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 40.91 % 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 2.5532e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NME, 6PG, 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	0.37	1/3536 (0.0%)	0.65	1/4789 (0.0%)
1	B	0.35	0/3533	0.66	1/4785 (0.0%)
1	C	0.38	1/3531 (0.0%)	0.65	2/4784 (0.0%)
1	D	0.35	0/3540	0.63	1/4795 (0.0%)
1	E	0.32	0/3517	0.63	0/4764
1	F	0.32	0/3540	0.63	0/4795
1	G	0.33	0/3517	0.66	1/4764 (0.0%)
1	H	0.31	0/3540	0.62	1/4795 (0.0%)
2	S	0.31	0/1048	0.61	0/1421
2	T	0.31	0/1048	0.59	0/1421
2	U	0.31	0/1048	0.60	0/1421
2	V	0.31	0/1048	0.61	0/1421
2	W	0.31	0/1048	0.61	0/1421
2	X	0.32	0/1048	0.61	0/1421
2	Y	0.31	0/1048	0.59	0/1421
2	Z	0.31	0/1048	0.59	0/1421
All	All	0.34	2/36638 (0.0%)	0.63	7/49639 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	GLY	N-CA	10.71	1.62	1.46
1	A	17	VAL	CB-CG1	5.68	1.64	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ALA	N-CA-C	6.63	128.90	111.00
1	C	13	PHE	N-CA-C	-6.62	93.14	111.00
1	G	15	ALA	N-CA-C	5.88	126.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	VAL	N-CA-C	5.49	125.81	111.00
1	C	13	PHE	N-CA-CB	5.17	119.91	110.60

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	3464	0	3370	79	0
1	B	3461	0	3369	109	0
1	C	3459	0	3365	102	0
1	D	3468	0	3378	74	0
1	E	3445	0	3347	74	0
1	F	3468	0	3378	85	0
1	G	3445	0	3347	95	0
1	H	3468	0	3378	78	0
2	S	1016	0	1017	41	0
2	T	1016	0	1017	36	0
2	U	1016	0	1017	33	0
2	V	1016	0	1017	43	0
2	W	1016	0	1017	50	0
2	X	1016	0	1017	44	0
2	Y	1016	0	1017	50	0
2	Z	1016	0	1017	48	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
4	A	17	0	9	0	0
4	B	17	0	9	0	0
4	C	17	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	17	0	9	0	0
4	E	17	0	9	0	0
4	F	17	0	9	0	0
4	G	17	0	9	0	0
4	H	17	0	9	0	0
5	A	309	0	0	23	0
5	B	345	0	0	32	0
5	C	339	0	0	47	0
5	D	335	0	0	14	0
5	E	318	0	0	22	0
5	F	371	0	0	34	0
5	G	341	0	0	26	0
5	H	326	0	0	27	0
5	S	113	0	0	11	0
5	T	99	0	0	13	0
5	U	125	0	0	8	0
5	V	123	0	0	12	0
5	W	122	0	0	13	0
5	X	115	0	0	19	0
5	Y	111	0	0	14	0
5	Z	115	0	0	10	0
All	All	39557	0	35140	978	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 14.

The worst 5 of 978 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HG2	5:A:480:HOH:O	1.42	1.16
1:E:358:ARG:HH21	1:E:358:ARG:HG3	0.98	1.09
1:D:16:GLY:HA2	1:D:68:THR:CB	1.83	1.08
1:C:330:THR:HG23	1:C:379:SER:O	1.56	1.04
1:G:15:ALA:HB1	5:G:591:HOH:O	1.56	1.04

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	437/477 (92%)	412 (94%)	20 (5%)	5 (1%)	17	3
1	B	436/477 (91%)	416 (95%)	18 (4%)	2 (0%)	32	12
1	C	436/477 (91%)	417 (96%)	17 (4%)	2 (0%)	32	12
1	D	437/477 (92%)	416 (95%)	20 (5%)	1 (0%)	51	28
1	E	434/477 (91%)	419 (96%)	15 (4%)	0	100	100
1	F	437/477 (92%)	415 (95%)	21 (5%)	1 (0%)	51	28
1	G	434/477 (91%)	415 (96%)	17 (4%)	2 (0%)	32	12
1	H	437/477 (92%)	415 (95%)	21 (5%)	1 (0%)	51	28
2	S	121/129 (94%)	113 (93%)	7 (6%)	1 (1%)	22	5
2	T	121/129 (94%)	114 (94%)	7 (6%)	0	100	100
2	U	121/129 (94%)	113 (93%)	8 (7%)	0	100	100
2	V	121/129 (94%)	112 (93%)	6 (5%)	3 (2%)	6	0
2	W	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
2	X	121/129 (94%)	111 (92%)	8 (7%)	2 (2%)	11	1
2	Y	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
2	Z	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
All	All	4456/4848 (92%)	4236 (95%)	200 (4%)	20 (0%)	38	17

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	333	GLY
2	S	120	PRO
1	C	331	VAL
1	D	15	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	355/385 (92%)	351 (99%)	4 (1%)	78	61
1	B	355/385 (92%)	352 (99%)	3 (1%)	85	73
1	C	355/385 (92%)	350 (99%)	5 (1%)	71	50
1	D	356/385 (92%)	354 (99%)	2 (1%)	89	79
1	E	353/385 (92%)	349 (99%)	4 (1%)	78	61
1	F	356/385 (92%)	352 (99%)	4 (1%)	78	61
1	G	353/385 (92%)	345 (98%)	8 (2%)	56	28
1	H	356/385 (92%)	354 (99%)	2 (1%)	89	79
2	S	110/114 (96%)	108 (98%)	2 (2%)	64	40
2	T	110/114 (96%)	108 (98%)	2 (2%)	64	40
2	U	110/114 (96%)	108 (98%)	2 (2%)	64	40
2	V	110/114 (96%)	108 (98%)	2 (2%)	64	40
2	W	110/114 (96%)	107 (97%)	3 (3%)	50	22
2	X	110/114 (96%)	108 (98%)	2 (2%)	64	40
2	Y	110/114 (96%)	109 (99%)	1 (1%)	82	69
2	Z	110/114 (96%)	108 (98%)	2 (2%)	64	40
All	All	3719/3992 (93%)	3671 (99%)	48 (1%)	73	54

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	112	LEU
2	W	21	LEU
1	H	297	MET
1	E	14	LYS
1	E	358	ARG

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

Mol	Chain	Res	Type
1	D	401	GLN
1	E	401	GLN
1	H	207	ASN
2	V	111	GLN
2	W	29	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	A	201	1,3	8,11,12	0.95	0	6,12,14	1.65	1 (16%)
1	KCX	B	201	1,3	8,11,12	1.07	1 (12%)	6,12,14	1.53	1 (16%)
1	KCX	C	201	1,3	8,11,12	0.95	0	6,12,14	1.42	1 (16%)
1	KCX	D	201	1,3	8,11,12	0.86	0	6,12,14	1.57	1 (16%)
1	KCX	E	201	1,3	8,11,12	0.88	0	6,12,14	1.44	1 (16%)
1	KCX	F	201	1,3	8,11,12	1.10	1 (12%)	6,12,14	1.56	1 (16%)
1	KCX	G	201	1,3	8,11,12	0.88	0	6,12,14	1.53	1 (16%)
1	KCX	H	201	1,3	8,11,12	0.95	0	6,12,14	1.50	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	201	1,3	-	0/6/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	F	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	G	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	H	201	1,3	-	0/6/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	KCX	CB-CA	2.12	1.56	1.53
1	F	201	KCX	CA-C	2.15	1.53	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	CB-CA-C	-3.55	105.80	111.65
1	D	201	KCX	CB-CA-C	-3.33	106.17	111.65
1	G	201	KCX	CB-CA-C	-3.30	106.22	111.65
1	B	201	KCX	CB-CA-C	-3.13	106.50	111.65
1	F	201	KCX	CB-CA-C	-3.10	106.53	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	6PG	A	479	3	13,16,16	1.11	2 (15%)	18,23,23	1.71	6 (33%)
4	6PG	B	479	3	13,16,16	1.37	1 (7%)	18,23,23	1.92	7 (38%)
4	6PG	C	479	3	13,16,16	1.07	1 (7%)	18,23,23	1.61	5 (27%)
4	6PG	D	479	3	13,16,16	1.36	1 (7%)	18,23,23	1.88	5 (27%)
4	6PG	E	479	3	13,16,16	1.11	2 (15%)	18,23,23	1.93	5 (27%)
4	6PG	F	479	3	13,16,16	1.15	1 (7%)	18,23,23	1.64	4 (22%)
4	6PG	G	479	3	13,16,16	1.15	2 (15%)	18,23,23	1.56	4 (22%)
4	6PG	H	479	3	13,16,16	1.31	1 (7%)	18,23,23	1.84	6 (33%)

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	6PG	A	479	3	-	0/18/22/22	0/0/0/0
4	6PG	B	479	3	-	0/18/22/22	0/0/0/0
4	6PG	C	479	3	-	0/18/22/22	0/0/0/0
4	6PG	D	479	3	-	0/18/22/22	0/0/0/0
4	6PG	E	479	3	-	0/18/22/22	0/0/0/0
4	6PG	F	479	3	-	0/18/22/22	0/0/0/0
4	6PG	G	479	3	-	0/18/22/22	0/0/0/0
4	6PG	H	479	3	-	0/18/22/22	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	479	6PG	P-O2P	-2.84	1.43	1.54
4	E	479	6PG	P-O3P	-2.46	1.44	1.54
4	D	479	6PG	P-O2P	-2.32	1.45	1.54
4	H	479	6PG	P-O2P	-2.31	1.45	1.54
4	F	479	6PG	P-O3P	-2.25	1.45	1.54

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	479	6PG	O4-C4-C3	-3.73	100.53	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	479	6PG	O4-C4-C3	-3.46	101.18	109.46
4	E	479	6PG	O6-P-O1P	-3.04	97.93	106.47
4	B	479	6PG	O3P-P-O6	-2.84	99.17	106.73
4	H	479	6PG	O6-P-O1P	-2.80	98.62	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	443/477 (92%)	-0.22	17 (3%)	41 43	7, 12, 29, 63	0
1	B	442/477 (92%)	-0.16	20 (4%)	34 34	7, 11, 29, 66	0
1	C	442/477 (92%)	-0.21	21 (4%)	31 30	7, 11, 29, 63	0
1	D	443/477 (92%)	-0.17	20 (4%)	34 34	6, 11, 30, 67	0
1	E	440/477 (92%)	-0.30	12 (2%)	55 57	6, 11, 29, 62	0
1	F	443/477 (92%)	-0.17	20 (4%)	34 34	7, 11, 30, 65	0
1	G	440/477 (92%)	-0.13	20 (4%)	34 34	7, 11, 27, 67	0
1	H	443/477 (92%)	-0.22	13 (2%)	52 54	7, 12, 30, 64	0
2	S	122/129 (94%)	0.02	5 (4%)	38 38	9, 15, 27, 59	0
2	T	122/129 (94%)	-0.08	6 (4%)	30 29	8, 15, 28, 55	0
2	U	122/129 (94%)	-0.15	5 (4%)	38 38	8, 14, 25, 53	0
2	V	122/129 (94%)	-0.07	6 (4%)	30 29	8, 15, 25, 61	0
2	W	122/129 (94%)	0.00	7 (5%)	24 23	8, 15, 28, 55	0
2	X	122/129 (94%)	-0.23	4 (3%)	47 49	8, 15, 26, 55	0
2	Y	122/129 (94%)	-0.03	5 (4%)	38 38	9, 15, 27, 55	0
2	Z	122/129 (94%)	-0.13	5 (4%)	38 38	9, 15, 27, 56	0
All	All	4512/4848 (93%)	-0.17	186 (4%)	38 38	6, 12, 29, 67	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	17	VAL	19.6
1	D	16	GLY	19.1
2	S	123	CYS	18.0
1	F	331	VAL	13.9
1	F	92	GLY	13.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	C	201	12/13	0.97	0.07	-	7,8,11,12	0
1	KCX	E	201	12/13	0.97	0.07	-	8,9,11,12	0
1	KCX	G	201	12/13	0.96	0.06	-	7,9,11,11	0
1	KCX	H	201	12/13	0.97	0.08	-	7,9,11,12	0
1	KCX	B	201	12/13	0.97	0.06	-	9,10,11,11	0
1	KCX	F	201	12/13	0.98	0.06	-	7,9,11,11	0
1	KCX	D	201	12/13	0.97	0.07	-	7,8,10,11	0
1	KCX	A	201	12/13	0.97	0.07	-	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	6PG	B	479	17/17	0.89	0.12	1.16	12,21,27,27	0
4	6PG	E	479	17/17	0.94	0.09	0.73	12,20,29,30	0
4	6PG	D	479	17/17	0.93	0.10	0.58	10,20,29,30	0
4	6PG	C	479	17/17	0.95	0.08	0.33	11,17,23,24	0
4	6PG	F	479	17/17	0.94	0.09	0.31	12,21,26,27	0
4	6PG	H	479	17/17	0.93	0.08	0.21	11,20,31,33	0
4	6PG	A	479	17/17	0.94	0.07	-0.19	12,17,29,30	0
4	6PG	G	479	17/17	0.95	0.08	-0.25	11,19,25,26	0
3	MG	A	478	1/1	0.99	0.06	-0.98	11,11,11,11	0
3	MG	E	478	1/1	1.00	0.03	-2.30	11,11,11,11	0
3	MG	G	478	1/1	1.00	0.03	-2.79	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	478	1/1	0.99	0.05	-3.51	10,10,10,10	0
3	MG	B	478	1/1	0.99	0.04	-4.16	10,10,10,10	0
3	MG	F	478	1/1	1.00	0.04	-4.53	9,9,9,9	0
3	MG	H	478	1/1	0.99	0.03	-5.29	11,11,11,11	0
3	MG	D	478	1/1	1.00	0.03	-10.28	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.