



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2016 – 05:36 AM EST

PDB ID : 5HAN
Title : Structure function studies of R. palustris RubisCO (S59F mutant; CABP-bound)
Authors : Arbing, M.A.; Leong, J.G.; Varaljay, V.A.; Satagopan, S.; North, J.A.; Tabita, F.R.
Deposited on : 2015-12-30
Resolution : 2.04 Å(reported)

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

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

A user guide is available at

<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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

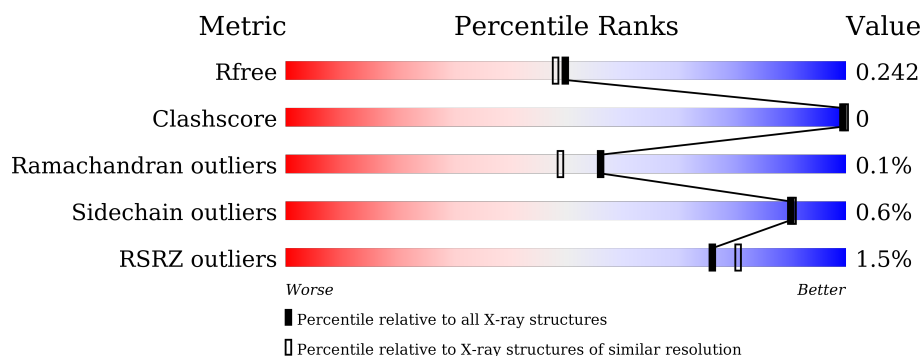
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	481	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>• 5%</div> </div> </div>
1	B	481	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>• 5%</div> </div> </div>
1	C	481	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>• 5%</div> </div> </div>
1	D	481	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>• 5%</div> </div> </div>
1	E	481	<div> <div></div> <div> <div></div> <div>94%</div> <div>• 5%</div> </div> </div>
1	F	481	<div> <div></div> <div> <div></div> <div>94%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	481	 <div>93% • 5%</div>
1	H	481	 <div>94% • 5%</div>
1	I	481	 <div>93% • 5%</div>
1	J	481	 <div>94% • 5%</div>
1	K	481	 <div>93% • 5%</div>
1	L	481	 <div>93% • 5%</div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 85695 atoms, of which 40512 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	0	0
			6906	2246	3377	610	654	19			
1	B	455	Total	C	H	N	O	S	0	0	0
			6857	2232	3346	607	653	19			
1	C	455	Total	C	H	N	O	S	0	0	0
			6891	2238	3371	609	654	19			
1	D	455	Total	C	H	N	O	S	0	0	0
			6906	2241	3382	610	654	19			
1	E	457	Total	C	H	N	O	S	0	0	0
			6892	2245	3363	610	655	19			
1	F	455	Total	C	H	N	O	S	0	0	0
			6898	2239	3378	610	652	19			
1	G	457	Total	C	H	N	O	S	0	0	0
			6892	2245	3363	610	655	19			
1	H	456	Total	C	H	N	O	S	0	0	0
			6898	2244	3370	610	655	19			
1	I	455	Total	C	H	N	O	S	0	0	0
			6876	2235	3360	608	654	19			
1	J	455	Total	C	H	N	O	S	0	0	0
			6879	2238	3359	609	654	19			
1	K	455	Total	C	H	N	O	S	0	0	0
			6866	2233	3357	607	650	19			
1	L	456	Total	C	H	N	O	S	0	0	0
			6907	2246	3378	610	654	19			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q6N0W9
A	-18	GLY	-	expression tag	UNP Q6N0W9
A	-17	SER	-	expression tag	UNP Q6N0W9
A	-16	SER	-	expression tag	UNP Q6N0W9
A	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q6N0W9
A	-13	HIS	-	expression tag	UNP Q6N0W9
A	-12	HIS	-	expression tag	UNP Q6N0W9
A	-11	HIS	-	expression tag	UNP Q6N0W9
A	-10	HIS	-	expression tag	UNP Q6N0W9
A	-9	SER	-	expression tag	UNP Q6N0W9
A	-8	SER	-	expression tag	UNP Q6N0W9
A	-7	GLY	-	expression tag	UNP Q6N0W9
A	-6	LEU	-	expression tag	UNP Q6N0W9
A	-5	VAL	-	expression tag	UNP Q6N0W9
A	-4	PRO	-	expression tag	UNP Q6N0W9
A	-3	ARG	-	expression tag	UNP Q6N0W9
A	-2	GLY	-	expression tag	UNP Q6N0W9
A	-1	SER	-	expression tag	UNP Q6N0W9
A	0	HIS	-	expression tag	UNP Q6N0W9
A	59	PHE	SER	engineered mutation	UNP Q6N0W9
B	-19	MET	-	initiating methionine	UNP Q6N0W9
B	-18	GLY	-	expression tag	UNP Q6N0W9
B	-17	SER	-	expression tag	UNP Q6N0W9
B	-16	SER	-	expression tag	UNP Q6N0W9
B	-15	HIS	-	expression tag	UNP Q6N0W9
B	-14	HIS	-	expression tag	UNP Q6N0W9
B	-13	HIS	-	expression tag	UNP Q6N0W9
B	-12	HIS	-	expression tag	UNP Q6N0W9
B	-11	HIS	-	expression tag	UNP Q6N0W9
B	-10	HIS	-	expression tag	UNP Q6N0W9
B	-9	SER	-	expression tag	UNP Q6N0W9
B	-8	SER	-	expression tag	UNP Q6N0W9
B	-7	GLY	-	expression tag	UNP Q6N0W9
B	-6	LEU	-	expression tag	UNP Q6N0W9
B	-5	VAL	-	expression tag	UNP Q6N0W9
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B	-1	SER	-	expression tag	UNP Q6N0W9
B	0	HIS	-	expression tag	UNP Q6N0W9
B	59	PHE	SER	engineered mutation	UNP Q6N0W9
C	-19	MET	-	initiating methionine	UNP Q6N0W9
C	-18	GLY	-	expression tag	UNP Q6N0W9
C	-17	SER	-	expression tag	UNP Q6N0W9
C	-16	SER	-	expression tag	UNP Q6N0W9
C	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q6N0W9
C	-13	HIS	-	expression tag	UNP Q6N0W9
C	-12	HIS	-	expression tag	UNP Q6N0W9
C	-11	HIS	-	expression tag	UNP Q6N0W9
C	-10	HIS	-	expression tag	UNP Q6N0W9
C	-9	SER	-	expression tag	UNP Q6N0W9
C	-8	SER	-	expression tag	UNP Q6N0W9
C	-7	GLY	-	expression tag	UNP Q6N0W9
C	-6	LEU	-	expression tag	UNP Q6N0W9
C	-5	VAL	-	expression tag	UNP Q6N0W9
C	-4	PRO	-	expression tag	UNP Q6N0W9
C	-3	ARG	-	expression tag	UNP Q6N0W9
C	-2	GLY	-	expression tag	UNP Q6N0W9
C	-1	SER	-	expression tag	UNP Q6N0W9
C	0	HIS	-	expression tag	UNP Q6N0W9
C	59	PHE	SER	engineered mutation	UNP Q6N0W9
D	-19	MET	-	initiating methionine	UNP Q6N0W9
D	-18	GLY	-	expression tag	UNP Q6N0W9
D	-17	SER	-	expression tag	UNP Q6N0W9
D	-16	SER	-	expression tag	UNP Q6N0W9
D	-15	HIS	-	expression tag	UNP Q6N0W9
D	-14	HIS	-	expression tag	UNP Q6N0W9
D	-13	HIS	-	expression tag	UNP Q6N0W9
D	-12	HIS	-	expression tag	UNP Q6N0W9
D	-11	HIS	-	expression tag	UNP Q6N0W9
D	-10	HIS	-	expression tag	UNP Q6N0W9
D	-9	SER	-	expression tag	UNP Q6N0W9
D	-8	SER	-	expression tag	UNP Q6N0W9
D	-7	GLY	-	expression tag	UNP Q6N0W9
D	-6	LEU	-	expression tag	UNP Q6N0W9
D	-5	VAL	-	expression tag	UNP Q6N0W9
D	-4	PRO	-	expression tag	UNP Q6N0W9
D	-3	ARG	-	expression tag	UNP Q6N0W9
D	-2	GLY	-	expression tag	UNP Q6N0W9
D	-1	SER	-	expression tag	UNP Q6N0W9
D	0	HIS	-	expression tag	UNP Q6N0W9
D	59	PHE	SER	engineered mutation	UNP Q6N0W9
E	-19	MET	-	initiating methionine	UNP Q6N0W9
E	-18	GLY	-	expression tag	UNP Q6N0W9
E	-17	SER	-	expression tag	UNP Q6N0W9
E	-16	SER	-	expression tag	UNP Q6N0W9
E	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP Q6N0W9
E	-13	HIS	-	expression tag	UNP Q6N0W9
E	-12	HIS	-	expression tag	UNP Q6N0W9
E	-11	HIS	-	expression tag	UNP Q6N0W9
E	-10	HIS	-	expression tag	UNP Q6N0W9
E	-9	SER	-	expression tag	UNP Q6N0W9
E	-8	SER	-	expression tag	UNP Q6N0W9
E	-7	GLY	-	expression tag	UNP Q6N0W9
E	-6	LEU	-	expression tag	UNP Q6N0W9
E	-5	VAL	-	expression tag	UNP Q6N0W9
E	-4	PRO	-	expression tag	UNP Q6N0W9
E	-3	ARG	-	expression tag	UNP Q6N0W9
E	-2	GLY	-	expression tag	UNP Q6N0W9
E	-1	SER	-	expression tag	UNP Q6N0W9
E	0	HIS	-	expression tag	UNP Q6N0W9
E	59	PHE	SER	engineered mutation	UNP Q6N0W9
F	-19	MET	-	initiating methionine	UNP Q6N0W9
F	-18	GLY	-	expression tag	UNP Q6N0W9
F	-17	SER	-	expression tag	UNP Q6N0W9
F	-16	SER	-	expression tag	UNP Q6N0W9
F	-15	HIS	-	expression tag	UNP Q6N0W9
F	-14	HIS	-	expression tag	UNP Q6N0W9
F	-13	HIS	-	expression tag	UNP Q6N0W9
F	-12	HIS	-	expression tag	UNP Q6N0W9
F	-11	HIS	-	expression tag	UNP Q6N0W9
F	-10	HIS	-	expression tag	UNP Q6N0W9
F	-9	SER	-	expression tag	UNP Q6N0W9
F	-8	SER	-	expression tag	UNP Q6N0W9
F	-7	GLY	-	expression tag	UNP Q6N0W9
F	-6	LEU	-	expression tag	UNP Q6N0W9
F	-5	VAL	-	expression tag	UNP Q6N0W9
F	-4	PRO	-	expression tag	UNP Q6N0W9
F	-3	ARG	-	expression tag	UNP Q6N0W9
F	-2	GLY	-	expression tag	UNP Q6N0W9
F	-1	SER	-	expression tag	UNP Q6N0W9
F	0	HIS	-	expression tag	UNP Q6N0W9
F	59	PHE	SER	engineered mutation	UNP Q6N0W9
G	-19	MET	-	initiating methionine	UNP Q6N0W9
G	-18	GLY	-	expression tag	UNP Q6N0W9
G	-17	SER	-	expression tag	UNP Q6N0W9
G	-16	SER	-	expression tag	UNP Q6N0W9
G	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP Q6N0W9
G	-13	HIS	-	expression tag	UNP Q6N0W9
G	-12	HIS	-	expression tag	UNP Q6N0W9
G	-11	HIS	-	expression tag	UNP Q6N0W9
G	-10	HIS	-	expression tag	UNP Q6N0W9
G	-9	SER	-	expression tag	UNP Q6N0W9
G	-8	SER	-	expression tag	UNP Q6N0W9
G	-7	GLY	-	expression tag	UNP Q6N0W9
G	-6	LEU	-	expression tag	UNP Q6N0W9
G	-5	VAL	-	expression tag	UNP Q6N0W9
G	-4	PRO	-	expression tag	UNP Q6N0W9
G	-3	ARG	-	expression tag	UNP Q6N0W9
G	-2	GLY	-	expression tag	UNP Q6N0W9
G	-1	SER	-	expression tag	UNP Q6N0W9
G	0	HIS	-	expression tag	UNP Q6N0W9
G	59	PHE	SER	engineered mutation	UNP Q6N0W9
H	-19	MET	-	initiating methionine	UNP Q6N0W9
H	-18	GLY	-	expression tag	UNP Q6N0W9
H	-17	SER	-	expression tag	UNP Q6N0W9
H	-16	SER	-	expression tag	UNP Q6N0W9
H	-15	HIS	-	expression tag	UNP Q6N0W9
H	-14	HIS	-	expression tag	UNP Q6N0W9
H	-13	HIS	-	expression tag	UNP Q6N0W9
H	-12	HIS	-	expression tag	UNP Q6N0W9
H	-11	HIS	-	expression tag	UNP Q6N0W9
H	-10	HIS	-	expression tag	UNP Q6N0W9
H	-9	SER	-	expression tag	UNP Q6N0W9
H	-8	SER	-	expression tag	UNP Q6N0W9
H	-7	GLY	-	expression tag	UNP Q6N0W9
H	-6	LEU	-	expression tag	UNP Q6N0W9
H	-5	VAL	-	expression tag	UNP Q6N0W9
H	-4	PRO	-	expression tag	UNP Q6N0W9
H	-3	ARG	-	expression tag	UNP Q6N0W9
H	-2	GLY	-	expression tag	UNP Q6N0W9
H	-1	SER	-	expression tag	UNP Q6N0W9
H	0	HIS	-	expression tag	UNP Q6N0W9
H	59	PHE	SER	engineered mutation	UNP Q6N0W9
I	-19	MET	-	initiating methionine	UNP Q6N0W9
I	-18	GLY	-	expression tag	UNP Q6N0W9
I	-17	SER	-	expression tag	UNP Q6N0W9
I	-16	SER	-	expression tag	UNP Q6N0W9
I	-15	HIS	-	expression tag	UNP Q6N0W9

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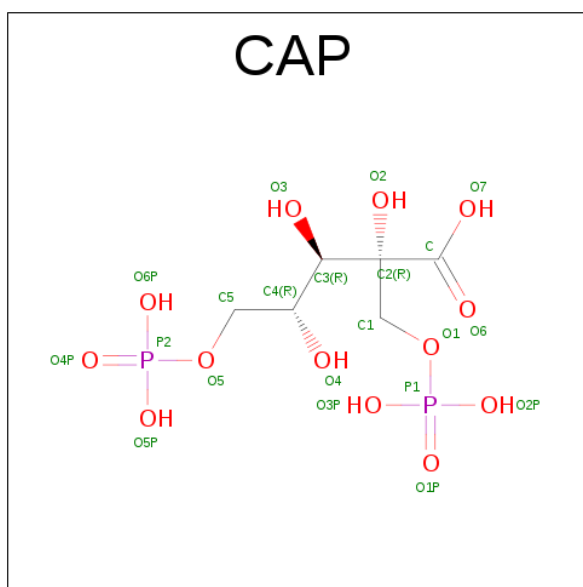
Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	expression tag	UNP Q6N0W9
I	-13	HIS	-	expression tag	UNP Q6N0W9
I	-12	HIS	-	expression tag	UNP Q6N0W9
I	-11	HIS	-	expression tag	UNP Q6N0W9
I	-10	HIS	-	expression tag	UNP Q6N0W9
I	-9	SER	-	expression tag	UNP Q6N0W9
I	-8	SER	-	expression tag	UNP Q6N0W9
I	-7	GLY	-	expression tag	UNP Q6N0W9
I	-6	LEU	-	expression tag	UNP Q6N0W9
I	-5	VAL	-	expression tag	UNP Q6N0W9
I	-4	PRO	-	expression tag	UNP Q6N0W9
I	-3	ARG	-	expression tag	UNP Q6N0W9
I	-2	GLY	-	expression tag	UNP Q6N0W9
I	-1	SER	-	expression tag	UNP Q6N0W9
I	0	HIS	-	expression tag	UNP Q6N0W9
I	59	PHE	SER	engineered mutation	UNP Q6N0W9
J	-19	MET	-	initiating methionine	UNP Q6N0W9
J	-18	GLY	-	expression tag	UNP Q6N0W9
J	-17	SER	-	expression tag	UNP Q6N0W9
J	-16	SER	-	expression tag	UNP Q6N0W9
J	-15	HIS	-	expression tag	UNP Q6N0W9
J	-14	HIS	-	expression tag	UNP Q6N0W9
J	-13	HIS	-	expression tag	UNP Q6N0W9
J	-12	HIS	-	expression tag	UNP Q6N0W9
J	-11	HIS	-	expression tag	UNP Q6N0W9
J	-10	HIS	-	expression tag	UNP Q6N0W9
J	-9	SER	-	expression tag	UNP Q6N0W9
J	-8	SER	-	expression tag	UNP Q6N0W9
J	-7	GLY	-	expression tag	UNP Q6N0W9
J	-6	LEU	-	expression tag	UNP Q6N0W9
J	-5	VAL	-	expression tag	UNP Q6N0W9
J	-4	PRO	-	expression tag	UNP Q6N0W9
J	-3	ARG	-	expression tag	UNP Q6N0W9
J	-2	GLY	-	expression tag	UNP Q6N0W9
J	-1	SER	-	expression tag	UNP Q6N0W9
J	0	HIS	-	expression tag	UNP Q6N0W9
J	59	PHE	SER	engineered mutation	UNP Q6N0W9
K	-19	MET	-	initiating methionine	UNP Q6N0W9
K	-18	GLY	-	expression tag	UNP Q6N0W9
K	-17	SER	-	expression tag	UNP Q6N0W9
K	-16	SER	-	expression tag	UNP Q6N0W9
K	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-14	HIS	-	expression tag	UNP Q6N0W9
K	-13	HIS	-	expression tag	UNP Q6N0W9
K	-12	HIS	-	expression tag	UNP Q6N0W9
K	-11	HIS	-	expression tag	UNP Q6N0W9
K	-10	HIS	-	expression tag	UNP Q6N0W9
K	-9	SER	-	expression tag	UNP Q6N0W9
K	-8	SER	-	expression tag	UNP Q6N0W9
K	-7	GLY	-	expression tag	UNP Q6N0W9
K	-6	LEU	-	expression tag	UNP Q6N0W9
K	-5	VAL	-	expression tag	UNP Q6N0W9
K	-4	PRO	-	expression tag	UNP Q6N0W9
K	-3	ARG	-	expression tag	UNP Q6N0W9
K	-2	GLY	-	expression tag	UNP Q6N0W9
K	-1	SER	-	expression tag	UNP Q6N0W9
K	0	HIS	-	expression tag	UNP Q6N0W9
K	59	PHE	SER	engineered mutation	UNP Q6N0W9
L	-19	MET	-	initiating methionine	UNP Q6N0W9
L	-18	GLY	-	expression tag	UNP Q6N0W9
L	-17	SER	-	expression tag	UNP Q6N0W9
L	-16	SER	-	expression tag	UNP Q6N0W9
L	-15	HIS	-	expression tag	UNP Q6N0W9
L	-14	HIS	-	expression tag	UNP Q6N0W9
L	-13	HIS	-	expression tag	UNP Q6N0W9
L	-12	HIS	-	expression tag	UNP Q6N0W9
L	-11	HIS	-	expression tag	UNP Q6N0W9
L	-10	HIS	-	expression tag	UNP Q6N0W9
L	-9	SER	-	expression tag	UNP Q6N0W9
L	-8	SER	-	expression tag	UNP Q6N0W9
L	-7	GLY	-	expression tag	UNP Q6N0W9
L	-6	LEU	-	expression tag	UNP Q6N0W9
L	-5	VAL	-	expression tag	UNP Q6N0W9
L	-4	PRO	-	expression tag	UNP Q6N0W9
L	-3	ARG	-	expression tag	UNP Q6N0W9
L	-2	GLY	-	expression tag	UNP Q6N0W9
L	-1	SER	-	expression tag	UNP Q6N0W9
L	0	HIS	-	expression tag	UNP Q6N0W9
L	59	PHE	SER	engineered mutation	UNP Q6N0W9

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C₆H₁₄O₁₃P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	B	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	C	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	D	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	E	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	F	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	G	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	H	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	I	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	J	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	K	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	L	1	Total	C	H	O	P	0	0
			30	6	9	13	2		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	235	Total O 235 235	0	0
4	B	196	Total O 196 196	0	0
4	C	213	Total O 213 213	0	0
4	D	214	Total O 214 214	0	0
4	E	241	Total O 241 241	0	0
4	F	284	Total O 284 284	0	0
4	G	217	Total O 217 217	0	0
4	H	230	Total O 230 230	0	0

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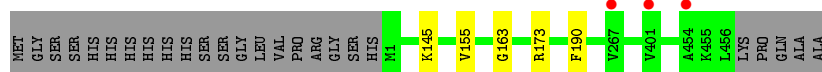
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	228	Total 228	O 228	0	0
4	J	172	Total 172	O 172	0	0
4	K	191	Total 191	O 191	0	0
4	L	234	Total 234	O 234	0	0

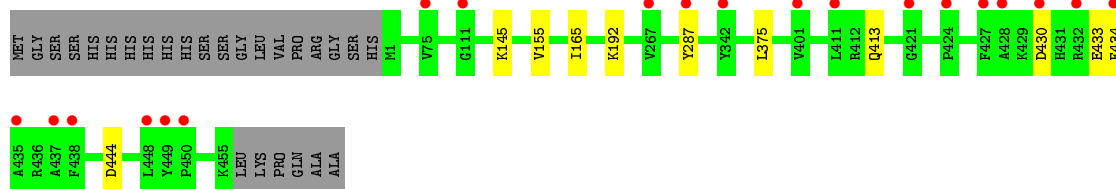
3 Residue-property plots [i](#)

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

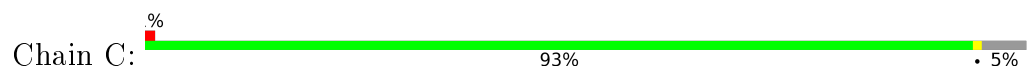
- Molecule 1: Ribulose biphosphate carboxylase



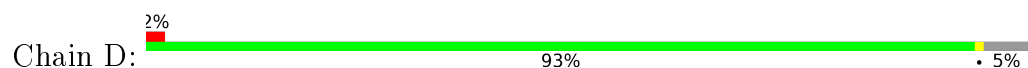
- Molecule 1: Ribulose biphosphate carboxylase



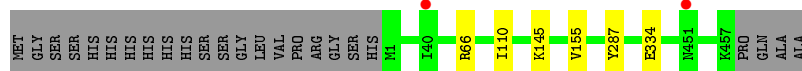
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase

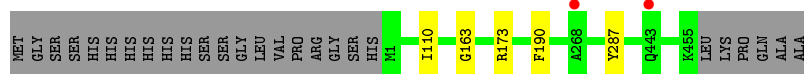


- Molecule 1: Ribulose biphosphate carboxylase




- Molecule 1: Ribulose biphosphate carboxylase

Chain F:  94% • 5%



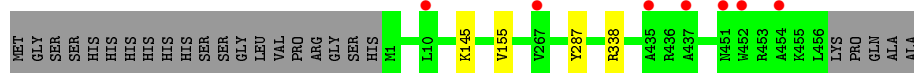
- Molecule 1: Ribulose biphosphate carboxylase

Chain G:  93% • 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain H:  94% • 5%



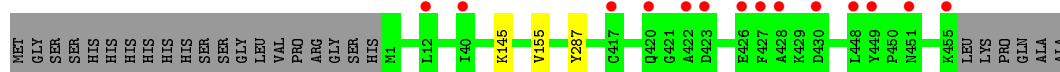
- Molecule 1: Ribulose biphosphate carboxylase

Chain I:  93% • 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain J:  94% • 5%



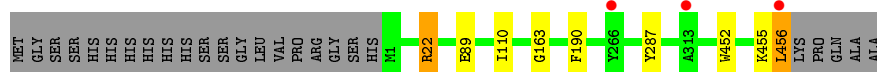
- Molecule 1: Ribulose biphosphate carboxylase

Chain K:  93% • 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain L:  93% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.88Å 110.37Å 167.36Å 89.87° 101.70° 105.00°	Depositor
Resolution (Å)	20.00 – 2.04 48.92 – 2.04	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.00-2.04) 87.8 (48.92-2.04)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.197 , 0.237 0.203 , 0.242	Depositor DCC
R_{free} test set	29077 reflections (11.11%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	85695	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 60.08 % 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 1.6054e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, CAP, 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	0.52	0/3606	0.63	0/4879
1	B	0.50	0/3588	0.63	0/4857
1	C	0.50	0/3597	0.63	0/4868
1	D	0.49	0/3601	0.63	0/4872
1	E	0.52	0/3606	0.64	0/4881
1	F	0.53	0/3597	0.64	0/4867
1	G	0.50	0/3606	0.64	0/4881
1	H	0.52	0/3605	0.63	0/4879
1	I	0.50	0/3593	0.62	0/4864
1	J	0.48	0/3597	0.63	0/4868
1	K	0.50	0/3586	0.63	0/4854
1	L	0.50	0/3606	0.64	0/4879
All	All	0.51	0/43188	0.63	0/58449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3529	3377	3401	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3511	3346	3361	6	0
1	C	3520	3371	3383	1	0
1	D	3524	3382	3394	1	0
1	E	3529	3363	3390	3	0
1	F	3520	3378	3390	1	0
1	G	3529	3363	3390	5	0
1	H	3528	3370	3394	2	0
1	I	3516	3360	3372	4	0
1	J	3520	3359	3383	1	0
1	K	3509	3357	3369	1	0
1	L	3529	3378	3401	4	0
2	A	21	9	7	0	0
2	B	21	9	8	0	0
2	C	21	9	7	0	0
2	D	21	9	7	0	0
2	E	21	9	7	0	0
2	F	21	9	7	0	0
2	G	21	9	7	0	0
2	H	21	9	7	0	0
2	I	21	9	7	0	0
2	J	21	9	7	0	0
2	K	21	9	7	0	0
2	L	21	9	7	0	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	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	235	0	0	1	0
4	B	196	0	0	0	0
4	C	213	0	0	0	0
4	D	214	0	0	0	0
4	E	241	0	0	2	0
4	F	284	0	0	0	0
4	G	217	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	230	0	0	0	0
4	I	228	0	0	0	0
4	J	172	0	0	0	0
4	K	191	0	0	0	0
4	L	234	0	0	0	0
All	All	45183	40512	40713	32	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 0.

All (32) 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:G:426:GLU:OE2	1:G:455:LYS:NZ	2.11	0.81
1:A:173:ARG:NH2	4:A:601:HOH:O	2.20	0.74
1:E:145:LYS:HG3	1:E:155:VAL:HB	1.69	0.72
1:G:10:LEU:HD11	1:G:40:ILE:HD12	1.82	0.61
1:I:31:LYS:CD	1:I:121:TYR:OH	2.56	0.53
1:J:145:LYS:HG2	1:J:155:VAL:O	2.08	0.53
1:B:145:LYS:HG3	1:B:155:VAL:HB	1.91	0.53
1:H:145:LYS:HG3	1:H:155:VAL:HB	1.91	0.51
1:L:455:LYS:O	1:L:456:LEU:HG	2.12	0.50
1:G:342:TYR:OH	1:G:384:LEU:O	2.20	0.49
1:H:145:LYS:CG	1:H:155:VAL:HB	2.44	0.48
1:B:145:LYS:CG	1:B:155:VAL:HB	2.44	0.48
1:E:66:ARG:NH2	4:E:608:HOH:O	2.48	0.46
1:B:413:GLN:OE1	1:B:434:PHE:N	2.49	0.46
1:B:375:LEU:HD12	1:B:444:ASP:HB2	1.98	0.45
1:D:342:TYR:OH	1:D:384:LEU:O	2.30	0.45
1:E:334:GLU:HG2	4:E:682:HOH:O	2.16	0.45
1:A:163:GLY:HA2	1:A:190:PHE:O	2.17	0.45
1:G:451:ASN:O	1:G:455:LYS:HG3	2.17	0.44
1:I:31:LYS:HD2	1:I:121:TYR:OH	2.17	0.44
1:I:31:LYS:HD3	1:I:121:TYR:OH	2.18	0.43
1:B:433:GLU:OE1	1:B:433:GLU:N	2.50	0.43
1:C:145:LYS:HG2	1:C:155:VAL:O	2.20	0.42
1:B:165:ILE:HG12	1:B:192:KCX:HD2	2.02	0.42
1:F:163:GLY:HA2	1:F:190:PHE:O	2.20	0.42
1:G:145:LYS:HG2	1:G:155:VAL:O	2.19	0.42
1:L:22:ARG:NH1	1:L:89:GLU:OE2	2.52	0.42
1:L:163:GLY:HA2	1:L:190:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:GLY:HA2	1:I:190:PHE:O	2.21	0.41
1:A:145:LYS:HG2	1:A:155:VAL:O	2.21	0.41
1:K:342:TYR:OH	1:K:384:LEU:O	2.30	0.41
1:L:452:TRP:O	1:L:455:LYS:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	B	452/481 (94%)	441 (98%)	11 (2%)	0	100	100
1	C	452/481 (94%)	441 (98%)	11 (2%)	0	100	100
1	D	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	52	43
1	E	454/481 (94%)	443 (98%)	10 (2%)	1 (0%)	52	43
1	F	452/481 (94%)	441 (98%)	10 (2%)	1 (0%)	52	43
1	G	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	52	43
1	H	453/481 (94%)	442 (98%)	11 (2%)	0	100	100
1	I	452/481 (94%)	442 (98%)	9 (2%)	1 (0%)	52	43
1	J	452/481 (94%)	442 (98%)	10 (2%)	0	100	100
1	K	452/481 (94%)	439 (97%)	13 (3%)	0	100	100
1	L	453/481 (94%)	441 (97%)	11 (2%)	1 (0%)	52	43
All	All	5431/5772 (94%)	5294 (98%)	131 (2%)	6 (0%)	56	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	110	ILE
1	D	110	ILE
1	G	110	ILE
1	I	110	ILE
1	L	110	ILE
1	E	110	ILE

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	351/372 (94%)	351 (100%)	0	100	100
1	B	347/372 (93%)	345 (99%)	2 (1%)	90	90
1	C	350/372 (94%)	346 (99%)	4 (1%)	80	79
1	D	351/372 (94%)	348 (99%)	3 (1%)	84	84
1	E	350/372 (94%)	349 (100%)	1 (0%)	94	95
1	F	350/372 (94%)	348 (99%)	2 (1%)	90	90
1	G	350/372 (94%)	348 (99%)	2 (1%)	90	90
1	H	351/372 (94%)	349 (99%)	2 (1%)	90	90
1	I	349/372 (94%)	347 (99%)	2 (1%)	90	90
1	J	350/372 (94%)	349 (100%)	1 (0%)	94	95
1	K	347/372 (93%)	343 (99%)	4 (1%)	78	76
1	L	351/372 (94%)	348 (99%)	3 (1%)	84	84
All	All	4197/4464 (94%)	4171 (99%)	26 (1%)	90	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	TYR
1	B	430	ASP
1	C	22	ARG
1	C	287	TYR
1	C	338	ARG

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Mol	Chain	Res	Type
1	C	455	LYS
1	D	173	ARG
1	D	287	TYR
1	D	455	LYS
1	E	287	TYR
1	F	173	ARG
1	F	287	TYR
1	G	287	TYR
1	G	451	ASN
1	H	287	TYR
1	H	338	ARG
1	I	287	TYR
1	I	439	GLU
1	J	287	TYR
1	K	33	LYS
1	K	287	TYR
1	K	419	LYS
1	K	430	ASP
1	L	22	ARG
1	L	287	TYR
1	L	456	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	192	1,3	6,11,12	1.12	0	7,12,14	1.72	2 (28%)
1	KCX	B	192	1,3	6,11,12	1.26	1 (16%)	7,12,14	1.61	2 (28%)
1	KCX	C	192	1,3	6,11,12	1.30	0	7,12,14	1.28	1 (14%)
1	KCX	D	192	1,3	6,11,12	1.19	1 (16%)	7,12,14	1.28	1 (14%)
1	KCX	E	192	1,3	6,11,12	1.62	1 (16%)	7,12,14	1.70	2 (28%)
1	KCX	F	192	1,3	6,11,12	1.25	0	7,12,14	1.46	2 (28%)
1	KCX	G	192	1,3	6,11,12	0.84	0	7,12,14	1.57	2 (28%)
1	KCX	H	192	1,3	6,11,12	1.09	0	7,12,14	1.45	1 (14%)
1	KCX	I	192	1,3	6,11,12	0.95	0	7,12,14	1.40	1 (14%)
1	KCX	J	192	1,3	6,11,12	0.84	0	7,12,14	1.18	1 (14%)
1	KCX	K	192	1,3	6,11,12	2.03	1 (16%)	7,12,14	1.38	1 (14%)
1	KCX	L	192	1,3	6,11,12	1.73	1 (16%)	7,12,14	1.63	2 (28%)

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	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	F	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	G	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	H	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	I	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	J	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	K	192	1,3	-	0/6/10/12	0/0/0/0
1	KCX	L	192	1,3	-	0/6/10/12	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	192	KCX	CB-CA	-2.67	1.49	1.53
1	B	192	KCX	CB-CA	2.25	1.56	1.53
1	D	192	KCX	CE-NZ	2.46	1.51	1.46
1	L	192	KCX	CE-NZ	3.41	1.54	1.46
1	K	192	KCX	CE-NZ	4.31	1.56	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	KCX	CE-NZ-CX	-3.05	120.32	123.53
1	L	192	KCX	CE-NZ-CX	-2.96	120.42	123.53
1	G	192	KCX	CE-NZ-CX	-2.69	120.71	123.53
1	F	192	KCX	O-C-CA	-2.02	120.29	125.72
1	D	192	KCX	CB-CA-N	2.23	116.80	110.54
1	A	192	KCX	CB-CA-N	2.24	116.85	110.54
1	B	192	KCX	CE-NZ-CX	2.28	125.92	123.53
1	L	192	KCX	CB-CA-N	2.34	117.12	110.54
1	G	192	KCX	CB-CA-N	2.38	117.24	110.54
1	K	192	KCX	CB-CA-N	2.42	117.34	110.54
1	A	192	KCX	CE-NZ-CX	2.43	126.07	123.53
1	I	192	KCX	CB-CA-N	2.46	117.45	110.54
1	C	192	KCX	CB-CA-N	2.53	117.64	110.54
1	J	192	KCX	CB-CA-N	2.55	117.71	110.54
1	F	192	KCX	CB-CA-N	2.57	117.77	110.54
1	E	192	KCX	CB-CA-N	2.60	117.84	110.54
1	H	192	KCX	CB-CA-N	2.65	118.00	110.54
1	B	192	KCX	CD-CG-CB	2.66	123.11	113.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	192	KCX	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CAP	A	500	3	14,20,20	1.15	1 (7%)	16,31,31	1.57	3 (18%)
2	CAP	B	500	3	14,20,20	1.16	2 (14%)	16,31,31	1.76	5 (31%)
2	CAP	C	500	3	14,20,20	1.08	0	16,31,31	1.59	4 (25%)
2	CAP	D	500	3	14,20,20	1.03	0	16,31,31	1.61	4 (25%)
2	CAP	E	500	3	14,20,20	1.30	1 (7%)	16,31,31	1.60	5 (31%)
2	CAP	F	500	3	14,20,20	1.24	3 (21%)	16,31,31	1.47	3 (18%)
2	CAP	G	500	3	14,20,20	1.14	1 (7%)	16,31,31	1.67	6 (37%)
2	CAP	H	500	3	14,20,20	1.12	1 (7%)	16,31,31	1.69	6 (37%)
2	CAP	I	500	3	14,20,20	1.21	1 (7%)	16,31,31	1.62	4 (25%)
2	CAP	J	500	3	14,20,20	0.87	0	16,31,31	1.69	5 (31%)
2	CAP	K	500	3	14,20,20	1.01	1 (7%)	16,31,31	1.79	5 (31%)
2	CAP	L	500	3	14,20,20	1.08	0	16,31,31	1.66	5 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	A	500	3	-	0/23/29/29	0/0/0/0
2	CAP	B	500	3	-	0/23/29/29	0/0/0/0
2	CAP	C	500	3	-	0/23/29/29	0/0/0/0
2	CAP	D	500	3	-	0/23/29/29	0/0/0/0
2	CAP	E	500	3	-	0/23/29/29	0/0/0/0
2	CAP	F	500	3	-	0/23/29/29	0/0/0/0
2	CAP	G	500	3	-	0/23/29/29	0/0/0/0
2	CAP	H	500	3	-	0/23/29/29	0/0/0/0
2	CAP	I	500	3	-	0/23/29/29	0/0/0/0
2	CAP	J	500	3	-	0/23/29/29	0/0/0/0
2	CAP	K	500	3	-	0/23/29/29	0/0/0/0
2	CAP	L	500	3	-	0/23/29/29	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	CAP	P2-O6P	-2.78	1.45	1.54
2	G	500	CAP	P2-O6P	-2.55	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	CAP	P1-O2P	-2.44	1.46	1.54
2	E	500	CAP	O4-C4	-2.31	1.38	1.43
2	A	500	CAP	P2-O6P	-2.27	1.46	1.54
2	B	500	CAP	P2-O5P	-2.14	1.47	1.54
2	F	500	CAP	P2-O5P	-2.12	1.47	1.54
2	I	500	CAP	P1-O2P	-2.09	1.47	1.54
2	B	500	CAP	P2-O6P	-2.08	1.47	1.54
2	K	500	CAP	P2-O5P	-2.04	1.47	1.54
2	F	500	CAP	P2-O6P	-2.01	1.47	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	CAP	O3P-P1-O1P	-2.27	103.23	110.63
2	H	500	CAP	O3P-P1-O1P	-2.22	103.38	110.63
2	D	500	CAP	O3P-P1-O1P	-2.18	103.51	110.63
2	G	500	CAP	O3P-P1-O1P	-2.12	103.70	110.63
2	J	500	CAP	O3P-P1-O1P	-2.06	103.90	110.63
2	L	500	CAP	O3P-P1-O1P	-2.06	103.90	110.63
2	B	500	CAP	O3P-P1-O1P	-2.05	103.94	110.63
2	E	500	CAP	O6P-P2-O5	2.06	112.73	106.72
2	G	500	CAP	O1-P1-O1P	2.09	112.35	107.08
2	A	500	CAP	O3P-P1-O1	2.09	112.84	106.72
2	D	500	CAP	O1-P1-O1P	2.10	112.37	107.08
2	C	500	CAP	O2P-P1-O1	2.12	112.91	106.72
2	F	500	CAP	O3P-P1-O1	2.13	112.93	106.72
2	I	500	CAP	O6P-P2-O5	2.14	112.97	106.72
2	E	500	CAP	O1-P1-O1P	2.18	112.56	107.08
2	E	500	CAP	O3P-P1-O1	2.18	113.10	106.72
2	J	500	CAP	O2P-P1-O1	2.19	113.12	106.72
2	G	500	CAP	O2P-P1-O1	2.20	113.13	106.72
2	L	500	CAP	O2P-P1-O1	2.21	113.17	106.72
2	A	500	CAP	O6P-P2-O5	2.25	113.29	106.72
2	J	500	CAP	O1-P1-O1P	2.27	112.78	107.08
2	C	500	CAP	O6P-P2-O5	2.28	113.38	106.72
2	H	500	CAP	O1-P1-O1P	2.29	112.85	107.08
2	B	500	CAP	O1-P1-O1P	2.30	112.87	107.08
2	L	500	CAP	O1-P1-O1P	2.31	112.90	107.08
2	G	500	CAP	O3P-P1-O1	2.34	113.57	106.72
2	H	500	CAP	O6P-P2-O5	2.35	113.57	106.72
2	H	500	CAP	O5P-P2-O5	2.40	113.71	106.72
2	K	500	CAP	O1-P1-O1P	2.41	113.15	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	CAP	O5P-P2-O5	2.42	113.80	106.72
2	H	500	CAP	O2P-P1-O1	2.45	113.87	106.72
2	H	500	CAP	O3P-P1-O1	2.45	113.87	106.72
2	C	500	CAP	O3P-P1-O1	2.50	114.01	106.72
2	I	500	CAP	O2P-P1-O1	2.50	114.02	106.72
2	C	500	CAP	O5P-P2-O5	2.50	114.02	106.72
2	G	500	CAP	O6P-P2-O5	2.50	114.03	106.72
2	I	500	CAP	O3P-P1-O1	2.54	114.13	106.72
2	B	500	CAP	O3P-P1-O1	2.56	114.19	106.72
2	F	500	CAP	O5P-P2-O5	2.56	114.19	106.72
2	B	500	CAP	O5P-P2-O5	2.64	114.44	106.72
2	E	500	CAP	O2P-P1-O1	2.73	114.68	106.72
2	D	500	CAP	O3P-P1-O1	2.74	114.73	106.72
2	J	500	CAP	O5P-P2-O5	2.76	114.78	106.72
2	K	500	CAP	O2P-P1-O1	2.78	114.84	106.72
2	L	500	CAP	O3P-P1-O1	2.85	115.05	106.72
2	K	500	CAP	O5P-P2-O5	2.86	115.07	106.72
2	F	500	CAP	O2P-P1-O1	2.88	115.12	106.72
2	I	500	CAP	O5P-P2-O5	2.88	115.13	106.72
2	K	500	CAP	O3P-P1-O1	2.88	115.13	106.72
2	L	500	CAP	O5P-P2-O5	2.93	115.26	106.72
2	J	500	CAP	O3P-P1-O1	2.93	115.28	106.72
2	D	500	CAP	O5P-P2-O5	2.95	115.32	106.72
2	B	500	CAP	O2P-P1-O1	2.98	115.42	106.72
2	G	500	CAP	O5P-P2-O5	3.10	115.77	106.72
2	A	500	CAP	O5P-P2-O5	3.25	116.21	106.72

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/481 (94%)	0.01	3 (0%) 89 91	25, 36, 53, 68	0
1	B	454/481 (94%)	0.14	20 (4%) 38 43	26, 38, 61, 103	0
1	C	454/481 (94%)	-0.07	4 (0%) 85 89	27, 37, 55, 71	0
1	D	454/481 (94%)	-0.08	10 (2%) 65 71	24, 37, 55, 90	0
1	E	456/481 (94%)	-0.13	2 (0%) 93 94	24, 34, 50, 76	0
1	F	454/481 (94%)	-0.14	2 (0%) 93 94	24, 33, 48, 60	0
1	G	456/481 (94%)	-0.00	3 (0%) 89 91	26, 36, 52, 80	0
1	H	455/481 (94%)	-0.00	7 (1%) 76 81	25, 37, 53, 73	0
1	I	454/481 (94%)	-0.14	3 (0%) 89 91	25, 37, 55, 76	0
1	J	454/481 (94%)	0.01	14 (3%) 52 60	27, 39, 61, 107	0
1	K	454/481 (94%)	0.01	11 (2%) 62 68	27, 38, 60, 99	0
1	L	455/481 (94%)	-0.13	3 (0%) 89 91	28, 36, 53, 71	0
All	All	5455/5772 (94%)	-0.04	82 (1%) 76 81	24, 37, 56, 107	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	449	TYR	4.7
1	B	434	PHE	3.6
1	E	40	ILE	3.6
1	I	36	PHE	3.5
1	J	426	GLU	3.4
1	H	454	ALA	3.4
1	B	448	LEU	3.3
1	D	417	CYS	3.3
1	K	449	TYR	3.3
1	J	423	ASP	3.2
1	B	427	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	422	ALA	3.1
1	K	451	ASN	3.0
1	B	428	ALA	2.9
1	B	75	VAL	2.9
1	G	267	VAL	2.9
1	D	423	ASP	2.8
1	D	427	PHE	2.8
1	B	432	ARG	2.8
1	K	75	VAL	2.8
1	K	425	VAL	2.8
1	J	417	CYS	2.8
1	K	438	PHE	2.8
1	B	449	TYR	2.8
1	B	267	VAL	2.8
1	B	450	PRO	2.7
1	B	437	ALA	2.7
1	C	426	GLU	2.7
1	D	425	VAL	2.7
1	E	451	ASN	2.7
1	J	420	GLN	2.7
1	K	450	PRO	2.6
1	B	401	VAL	2.6
1	L	456	LEU	2.6
1	I	78	ALA	2.6
1	B	438	PHE	2.6
1	J	448	LEU	2.6
1	K	435	ALA	2.5
1	G	454	ALA	2.5
1	J	430	ASP	2.5
1	D	422	ALA	2.5
1	B	424	PRO	2.5
1	L	266	TYR	2.5
1	A	267	VAL	2.5
1	J	455	LYS	2.5
1	H	451	ASN	2.4
1	J	427	PHE	2.4
1	B	435	ALA	2.4
1	D	429	LYS	2.4
1	K	423	ASP	2.4
1	K	452	TRP	2.4
1	J	40	ILE	2.4
1	J	451	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	401	VAL	2.3
1	H	267	VAL	2.3
1	H	452	TRP	2.3
1	A	454	ALA	2.3
1	C	5	ASN	2.3
1	D	40	ILE	2.3
1	D	424	PRO	2.3
1	H	437	ALA	2.3
1	J	428	ALA	2.2
1	B	430	ASP	2.2
1	F	443	GLN	2.2
1	B	411	LEU	2.2
1	D	421	GLY	2.2
1	C	420	GLN	2.2
1	C	152	GLY	2.2
1	B	342	TYR	2.2
1	J	422	ALA	2.2
1	H	10	LEU	2.1
1	H	435	ALA	2.1
1	D	426	GLU	2.1
1	K	424	PRO	2.1
1	A	401	VAL	2.1
1	I	75	VAL	2.1
1	F	268	ALA	2.0
1	B	421	GLY	2.0
1	B	287	TYR	2.0
1	J	12	LEU	2.0
1	L	313	ALA	2.0
1	B	111	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	KCX	D	192	12/13	0.92	0.19	-	27,33,35,36	0
1	KCX	J	192	12/13	0.93	0.14	-	26,31,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	KCX	L	192	12/13	0.93	0.14	-	27,29,31,35	0
1	KCX	H	192	12/13	0.93	0.10	-	28,28,32,33	0
1	KCX	E	192	12/13	0.96	0.12	-	23,30,35,35	0
1	KCX	G	192	12/13	0.97	0.14	-	30,33,35,35	0
1	KCX	A	192	12/13	0.96	0.14	-	24,28,28,28	0
1	KCX	C	192	12/13	0.97	0.12	-	29,32,36,38	0
1	KCX	I	192	12/13	0.95	0.12	-	29,34,36,38	0
1	KCX	F	192	12/13	0.96	0.13	-	25,29,32,33	0
1	KCX	K	192	12/13	0.97	0.11	-	26,29,33,34	0
1	KCX	B	192	12/13	0.95	0.11	-	25,29,31,32	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
3	MG	H	501	1/1	0.98	0.13	1.01	33,33,33,33	0
2	CAP	C	500	21/21	0.98	0.13	0.82	31,36,42,46	0
2	CAP	B	500	21/21	0.97	0.13	0.62	30,33,39,48	0
3	MG	B	501	1/1	0.98	0.13	0.52	36,36,36,36	0
2	CAP	H	500	21/21	0.97	0.12	0.40	28,33,41,42	0
2	CAP	E	500	21/21	0.97	0.12	0.30	25,30,34,38	0
2	CAP	I	500	21/21	0.97	0.12	0.20	33,41,43,44	0
2	CAP	J	500	21/21	0.97	0.12	0.07	33,42,45,49	0
2	CAP	D	500	21/21	0.97	0.11	-0.14	30,34,38,42	0
2	CAP	A	500	21/21	0.97	0.11	-0.18	29,36,42,42	0
2	CAP	L	500	21/21	0.98	0.11	-0.20	30,34,40,41	0
2	CAP	K	500	21/21	0.98	0.11	-0.30	29,36,39,40	0
2	CAP	F	500	21/21	0.98	0.11	-0.36	25,33,42,43	0
3	MG	L	501	1/1	0.93	0.11	-0.47	32,32,32,32	0
2	CAP	G	500	21/21	0.96	0.10	-0.58	26,36,40,43	0
3	MG	I	501	1/1	0.94	0.09	-0.64	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	K	501	1/1	0.97	0.07	-1.93	30,30,30,30	0
3	MG	E	501	1/1	0.97	0.07	-1.96	25,25,25,25	0
3	MG	F	501	1/1	0.97	0.07	-1.99	32,32,32,32	0
3	MG	C	501	1/1	0.95	0.07	-2.09	34,34,34,34	0
3	MG	G	501	1/1	0.99	0.07	-2.19	33,33,33,33	0
3	MG	A	501	1/1	0.99	0.04	-2.90	30,30,30,30	0
3	MG	D	501	1/1	0.90	0.06	-3.18	35,35,35,35	0
3	MG	J	501	1/1	0.94	0.04	-3.75	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.