



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:23 am GMT

PDB ID : 3KDO  
Title : Crystal structure of Type III Rubisco SP6 mutant complexed with 2-CABP  
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2009-10-23  
Resolution : 2.36 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

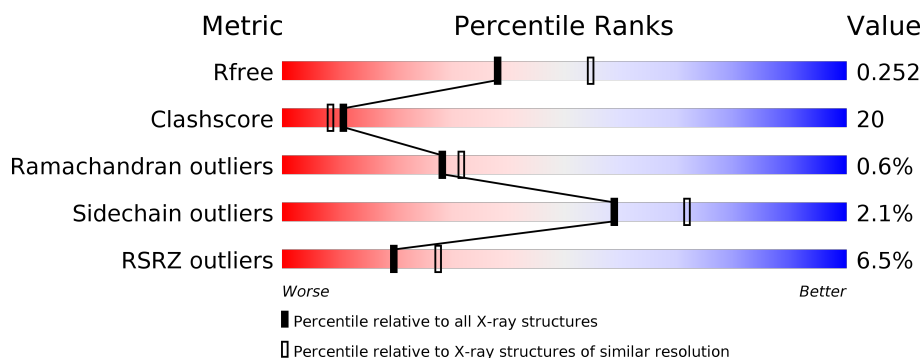
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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.



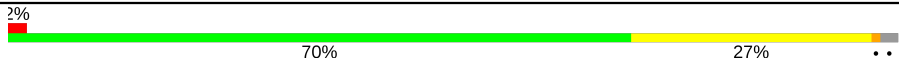

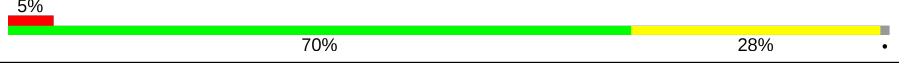
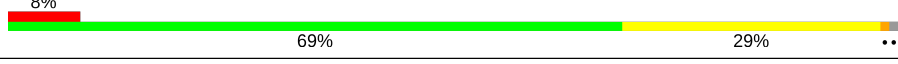
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	444	<div> <div>10%</div> <div>54%</div> <div>42%</div> <div>..</div> </div>
1	B	444	<div> <div>8%</div> <div>68%</div> <div>30%</div> <div>..</div> </div>
1	C	444	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
1	D	444	<div> <div>2%</div> <div>74%</div> <div>24%</div> <div>..</div> </div>
1	E	444	<div> <div>9%</div> <div>72%</div> <div>27%</div> <div>..</div> </div>
1	F	444	<div> <div>5%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36065 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3341	2146	569	616	10			
1	B	438	Total	C	N	O	S	0	0	0
			3391	2179	575	627	10			
1	C	440	Total	C	N	O	S	0	0	0
			3420	2196	580	634	10			
1	D	437	Total	C	N	O	S	0	0	0
			3419	2195	582	632	10			
1	E	440	Total	C	N	O	S	0	0	0
			3418	2198	582	628	10			
1	F	437	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			
1	G	437	Total	C	N	O	S	0	0	0
			3423	2200	582	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3382	2178	574	620	10			
1	I	438	Total	C	N	O	S	0	0	0
			3410	2190	582	628	10			
1	J	438	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	ENGINEERED	UNP O93627
A	327	ARG	LYS	ENGINEERED	UNP O93627
A	328	ASP	TRP	ENGINEERED	UNP O93627
A	329	ILE	ASP	ENGINEERED	UNP O93627
A	330	THR	VAL	ENGINEERED	UNP O93627
A	331	LEU	ILE	ENGINEERED	UNP O93627
A	332	GLY	GLN	ENGINEERED	UNP O93627
A	333	PHE	ASN	ENGINEERED	UNP O93627
A	334	VAL	ALA	ENGINEERED	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ARG	ENGINEERED	UNP O93627
A	336	LEU	ILE	ENGINEERED	UNP O93627
B	326	GLU	GLY	ENGINEERED	UNP O93627
B	327	ARG	LYS	ENGINEERED	UNP O93627
B	328	ASP	TRP	ENGINEERED	UNP O93627
B	329	ILE	ASP	ENGINEERED	UNP O93627
B	330	THR	VAL	ENGINEERED	UNP O93627
B	331	LEU	ILE	ENGINEERED	UNP O93627
B	332	GLY	GLN	ENGINEERED	UNP O93627
B	333	PHE	ASN	ENGINEERED	UNP O93627
B	334	VAL	ALA	ENGINEERED	UNP O93627
B	335	ASP	ARG	ENGINEERED	UNP O93627
B	336	LEU	ILE	ENGINEERED	UNP O93627
C	326	GLU	GLY	ENGINEERED	UNP O93627
C	327	ARG	LYS	ENGINEERED	UNP O93627
C	328	ASP	TRP	ENGINEERED	UNP O93627
C	329	ILE	ASP	ENGINEERED	UNP O93627
C	330	THR	VAL	ENGINEERED	UNP O93627
C	331	LEU	ILE	ENGINEERED	UNP O93627
C	332	GLY	GLN	ENGINEERED	UNP O93627
C	333	PHE	ASN	ENGINEERED	UNP O93627
C	334	VAL	ALA	ENGINEERED	UNP O93627
C	335	ASP	ARG	ENGINEERED	UNP O93627
C	336	LEU	ILE	ENGINEERED	UNP O93627
D	326	GLU	GLY	ENGINEERED	UNP O93627
D	327	ARG	LYS	ENGINEERED	UNP O93627
D	328	ASP	TRP	ENGINEERED	UNP O93627
D	329	ILE	ASP	ENGINEERED	UNP O93627
D	330	THR	VAL	ENGINEERED	UNP O93627
D	331	LEU	ILE	ENGINEERED	UNP O93627
D	332	GLY	GLN	ENGINEERED	UNP O93627
D	333	PHE	ASN	ENGINEERED	UNP O93627
D	334	VAL	ALA	ENGINEERED	UNP O93627
D	335	ASP	ARG	ENGINEERED	UNP O93627
D	336	LEU	ILE	ENGINEERED	UNP O93627
E	326	GLU	GLY	ENGINEERED	UNP O93627
E	327	ARG	LYS	ENGINEERED	UNP O93627
E	328	ASP	TRP	ENGINEERED	UNP O93627
E	329	ILE	ASP	ENGINEERED	UNP O93627
E	330	THR	VAL	ENGINEERED	UNP O93627
E	331	LEU	ILE	ENGINEERED	UNP O93627
E	332	GLY	GLN	ENGINEERED	UNP O93627

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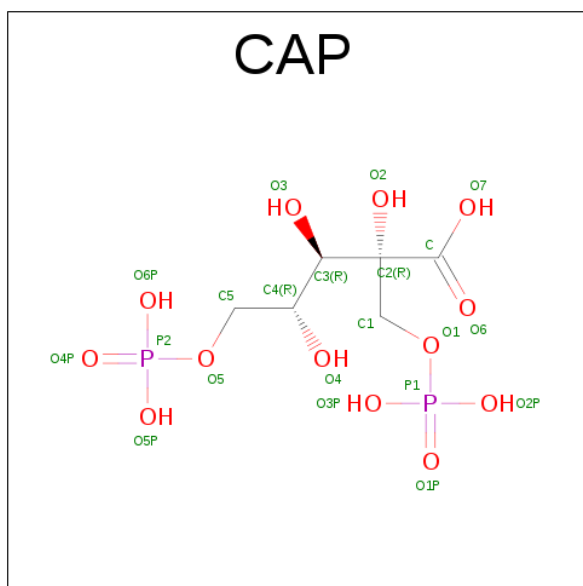
Chain	Residue	Modelled	Actual	Comment	Reference
E	333	PHE	ASN	ENGINEERED	UNP O93627
E	334	VAL	ALA	ENGINEERED	UNP O93627
E	335	ASP	ARG	ENGINEERED	UNP O93627
E	336	LEU	ILE	ENGINEERED	UNP O93627
F	326	GLU	GLY	ENGINEERED	UNP O93627
F	327	ARG	LYS	ENGINEERED	UNP O93627
F	328	ASP	TRP	ENGINEERED	UNP O93627
F	329	ILE	ASP	ENGINEERED	UNP O93627
F	330	THR	VAL	ENGINEERED	UNP O93627
F	331	LEU	ILE	ENGINEERED	UNP O93627
F	332	GLY	GLN	ENGINEERED	UNP O93627
F	333	PHE	ASN	ENGINEERED	UNP O93627
F	334	VAL	ALA	ENGINEERED	UNP O93627
F	335	ASP	ARG	ENGINEERED	UNP O93627
F	336	LEU	ILE	ENGINEERED	UNP O93627
G	326	GLU	GLY	ENGINEERED	UNP O93627
G	327	ARG	LYS	ENGINEERED	UNP O93627
G	328	ASP	TRP	ENGINEERED	UNP O93627
G	329	ILE	ASP	ENGINEERED	UNP O93627
G	330	THR	VAL	ENGINEERED	UNP O93627
G	331	LEU	ILE	ENGINEERED	UNP O93627
G	332	GLY	GLN	ENGINEERED	UNP O93627
G	333	PHE	ASN	ENGINEERED	UNP O93627
G	334	VAL	ALA	ENGINEERED	UNP O93627
G	335	ASP	ARG	ENGINEERED	UNP O93627
G	336	LEU	ILE	ENGINEERED	UNP O93627
H	326	GLU	GLY	ENGINEERED	UNP O93627
H	327	ARG	LYS	ENGINEERED	UNP O93627
H	328	ASP	TRP	ENGINEERED	UNP O93627
H	329	ILE	ASP	ENGINEERED	UNP O93627
H	330	THR	VAL	ENGINEERED	UNP O93627
H	331	LEU	ILE	ENGINEERED	UNP O93627
H	332	GLY	GLN	ENGINEERED	UNP O93627
H	333	PHE	ASN	ENGINEERED	UNP O93627
H	334	VAL	ALA	ENGINEERED	UNP O93627
H	335	ASP	ARG	ENGINEERED	UNP O93627
H	336	LEU	ILE	ENGINEERED	UNP O93627
I	326	GLU	GLY	ENGINEERED	UNP O93627
I	327	ARG	LYS	ENGINEERED	UNP O93627
I	328	ASP	TRP	ENGINEERED	UNP O93627
I	329	ILE	ASP	ENGINEERED	UNP O93627
I	330	THR	VAL	ENGINEERED	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
I	331	LEU	ILE	ENGINEERED	UNP O93627
I	332	GLY	GLN	ENGINEERED	UNP O93627
I	333	PHE	ASN	ENGINEERED	UNP O93627
I	334	VAL	ALA	ENGINEERED	UNP O93627
I	335	ASP	ARG	ENGINEERED	UNP O93627
I	336	LEU	ILE	ENGINEERED	UNP O93627
J	326	GLU	GLY	ENGINEERED	UNP O93627
J	327	ARG	LYS	ENGINEERED	UNP O93627
J	328	ASP	TRP	ENGINEERED	UNP O93627
J	329	ILE	ASP	ENGINEERED	UNP O93627
J	330	THR	VAL	ENGINEERED	UNP O93627
J	331	LEU	ILE	ENGINEERED	UNP O93627
J	332	GLY	GLN	ENGINEERED	UNP O93627
J	333	PHE	ASN	ENGINEERED	UNP O93627
J	334	VAL	ALA	ENGINEERED	UNP O93627
J	335	ASP	ARG	ENGINEERED	UNP O93627
J	336	LEU	ILE	ENGINEERED	UNP O93627

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



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

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

- 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	J	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	I	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 water.

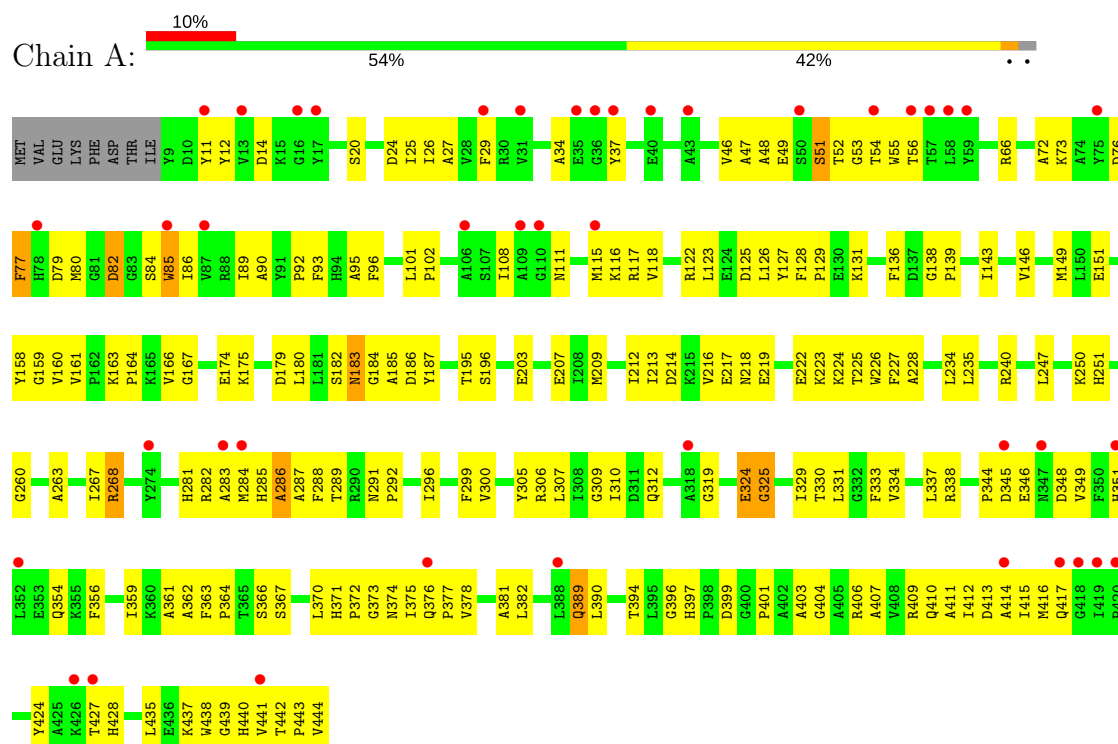


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total 97	O 97	0	0
4	B	175	Total 175	O 175	0	0
4	C	226	Total 226	O 226	0	0
4	D	239	Total 239	O 239	0	0
4	E	197	Total 197	O 197	0	0
4	F	179	Total 179	O 179	0	0
4	G	174	Total 174	O 174	0	0
4	H	123	Total 123	O 123	0	0
4	I	192	Total 192	O 192	0	0
4	J	209	Total 209	O 209	0	0

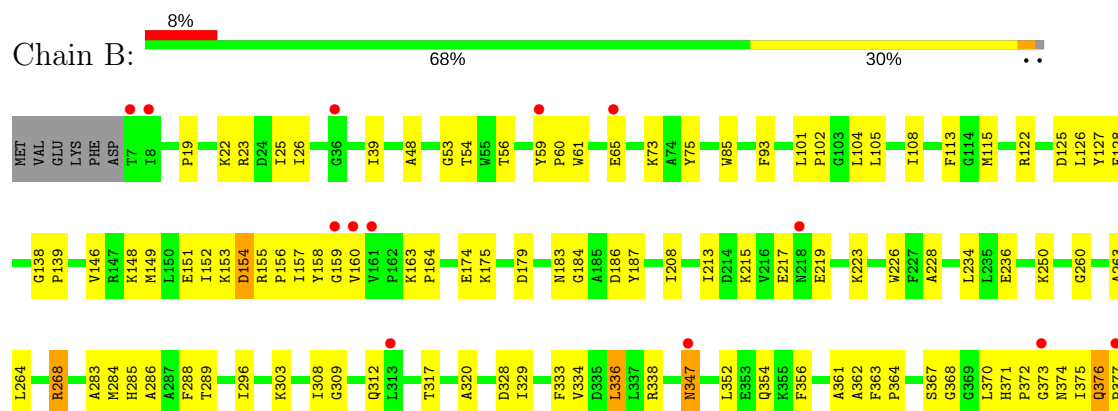
### 3 Residue-property plots

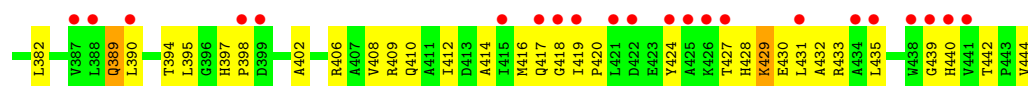
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Ribulose biphosphate carboxylase

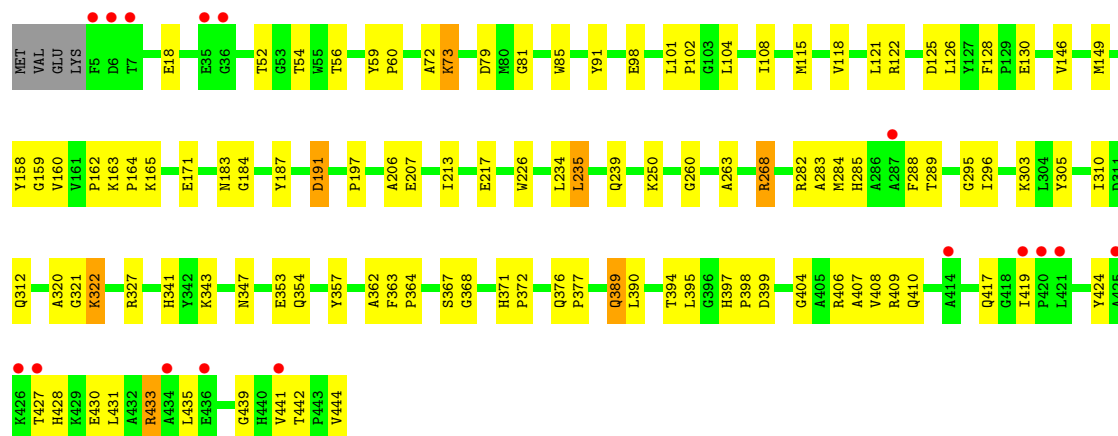
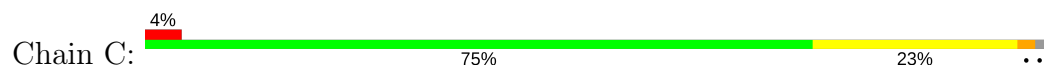


#### • Molecule 1: Ribulose biphosphate carboxylase

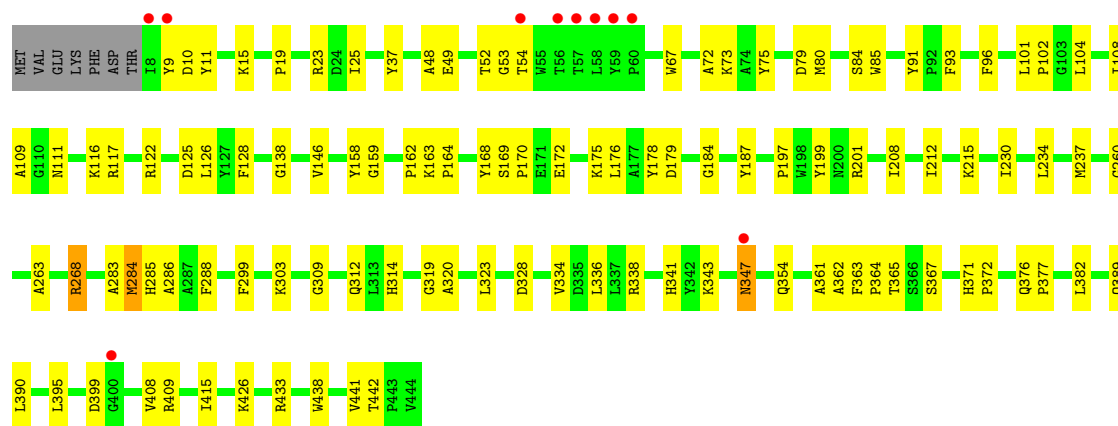
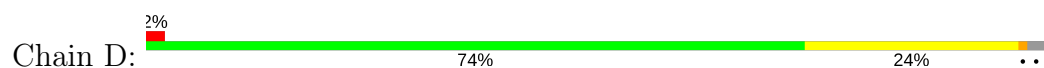




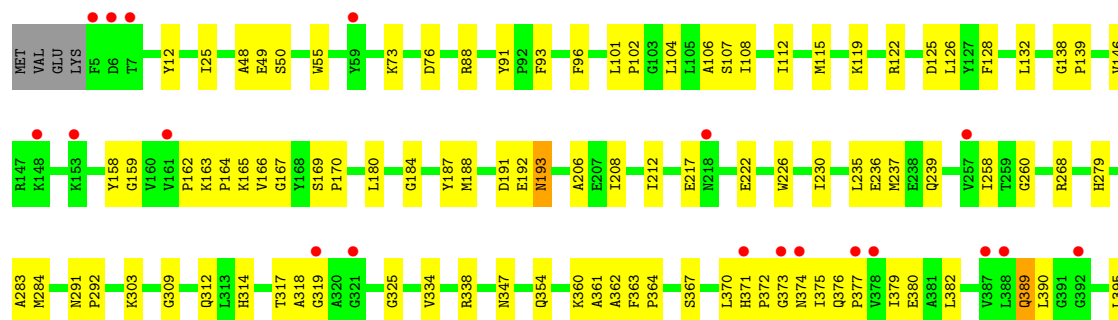
• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase

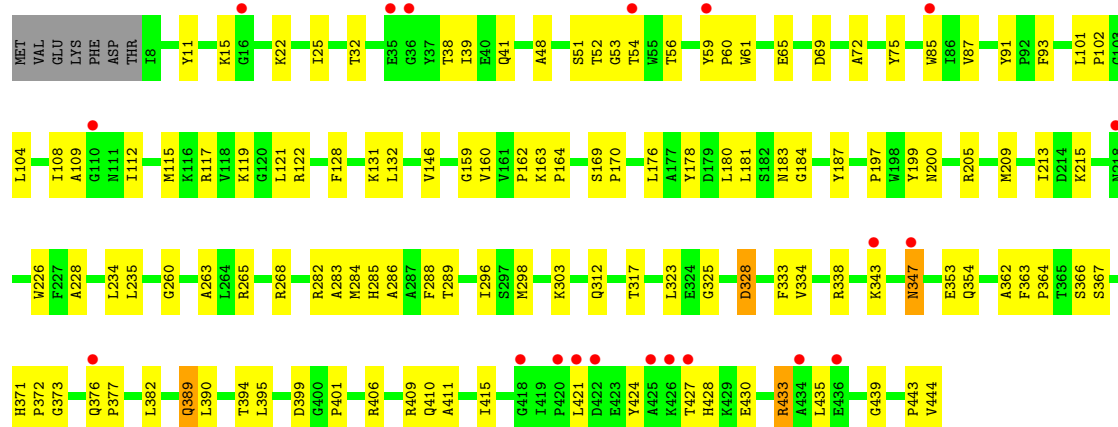


• Molecule 1: Ribulose biphosphate carboxylase

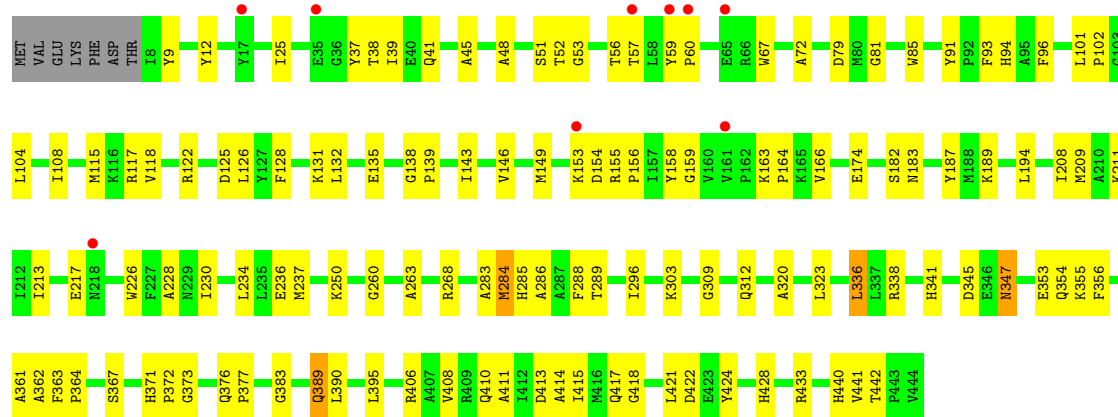




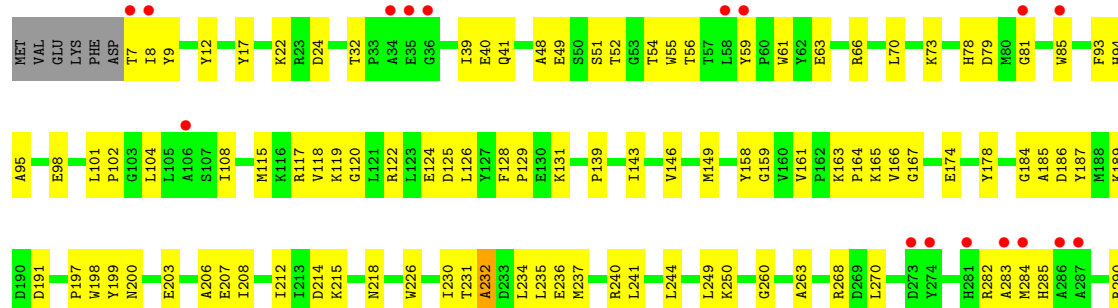
● Molecule 1: Ribulose biphosphate carboxylase

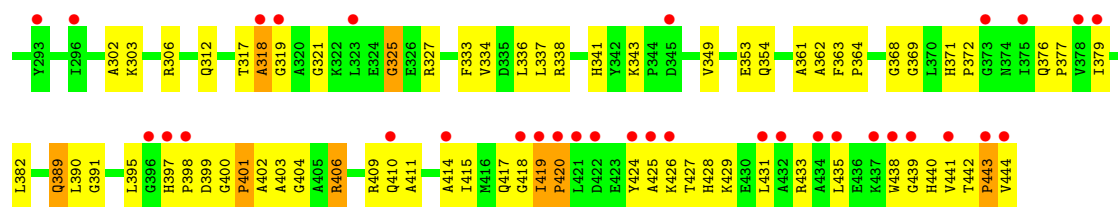


● Molecule 1: Ribulose biphosphate carboxylase

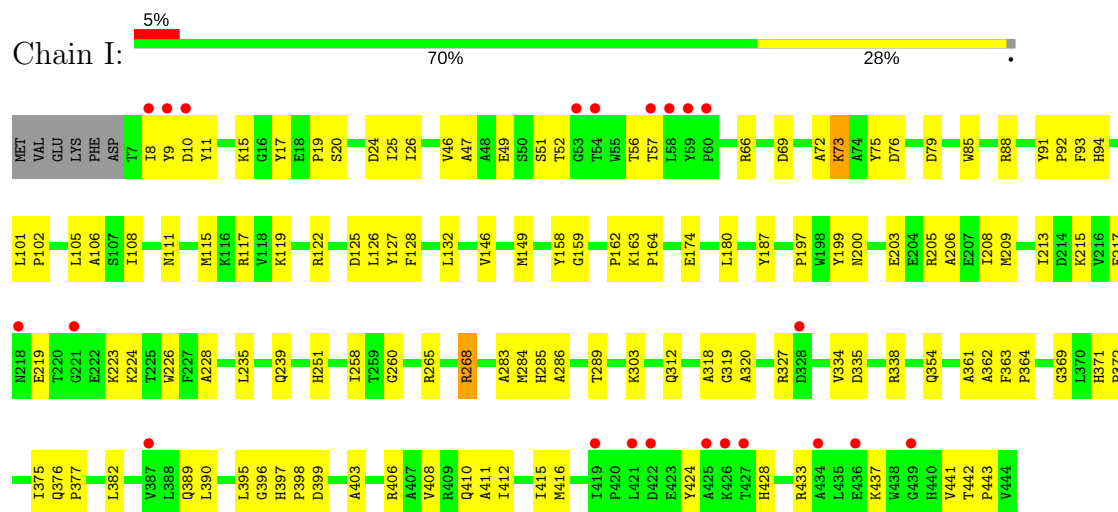


● Molecule 1: Ribulose biphosphate carboxylase

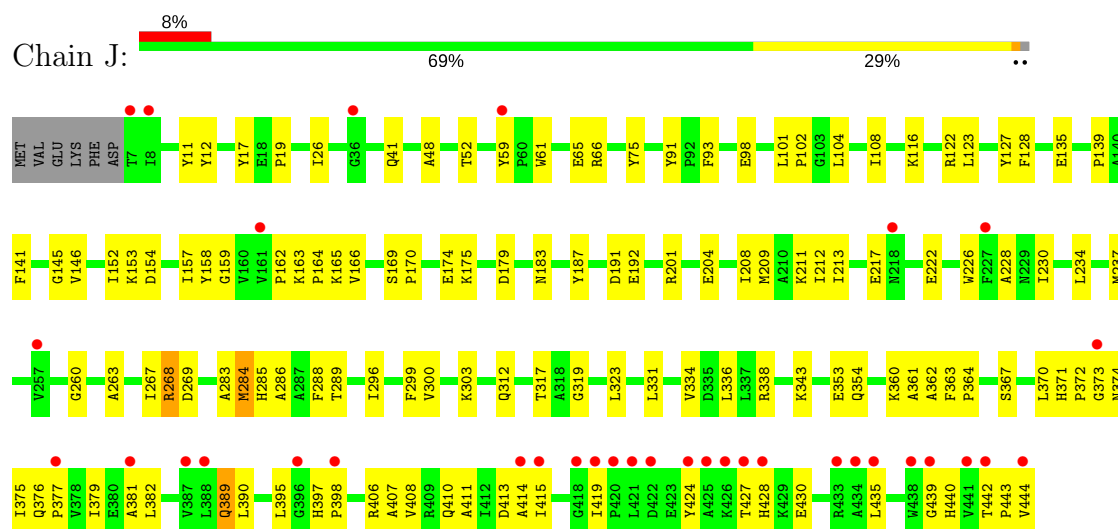




● Molecule 1: Ribulose biphosphate carboxylase



● Molecule 1: Ribulose biphosphate carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.48Å 246.57Å 134.83Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	38.46 – 2.36 38.46 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.46-2.36) 99.4 (38.46-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.219 , 0.264 0.213 , 0.252	Depositor DCC
$R_{free}$ test set	12530 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 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	0.21	0/3415	0.36	0/4642
1	B	0.22	0/3467	0.37	0/4712
1	C	0.22	0/3496	0.38	0/4750
1	D	0.22	0/3494	0.39	0/4739
1	E	0.22	0/3494	0.38	0/4744
1	F	0.22	0/3491	0.38	0/4738
1	G	0.21	0/3499	0.38	0/4747
1	H	0.21	0/3458	0.37	0/4700
1	I	0.22	0/3485	0.38	0/4730
1	J	0.22	0/3491	0.39	0/4738
All	All	0.22	0/34790	0.38	0/47240

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	3341	0	3185	218	0
1	B	3391	0	3252	153	0
1	C	3420	0	3289	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3419	0	3317	102	0
1	E	3418	0	3303	121	0
1	F	3415	0	3313	126	0
1	G	3423	0	3328	129	0
1	H	3382	0	3257	207	0
1	I	3410	0	3301	112	0
1	J	3415	0	3310	143	0
2	A	21	0	8	0	0
2	B	21	0	7	1	0
2	C	21	0	9	1	0
2	D	21	0	8	0	0
2	E	21	0	8	2	0
2	F	21	0	8	0	0
2	G	21	0	8	1	0
2	H	21	0	8	0	0
2	I	21	0	8	0	0
2	J	21	0	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
4	A	97	0	0	12	0
4	B	175	0	0	10	0
4	C	226	0	0	7	0
4	D	239	0	0	4	0
4	E	197	0	0	9	0
4	F	179	0	0	9	0
4	G	174	0	0	8	0
4	H	123	0	0	6	0
4	I	192	0	0	7	0
4	J	209	0	0	15	0
All	All	36065	0	32934	1362	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 20.

The worst 5 of 1362 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:H:397:HIS:ND1	1:H:398:PRO:HD2	1.29	1.44
1:H:397:HIS:CG	1:H:398:PRO:HD2	1.61	1.32
1:A:149:MET:HE3	1:A:250:LYS:CB	1.65	1.26
1:H:397:HIS:ND1	1:H:398:PRO:CD	2.06	1.18
1:I:72:ALA:O	1:I:73:LYS:HD2	1.43	1.17

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	433/444 (98%)	386 (89%)	40 (9%)	7 (2%)	11	9
1	B	435/444 (98%)	408 (94%)	25 (6%)	2 (0%)	32	37
1	C	437/444 (98%)	420 (96%)	16 (4%)	1 (0%)	51	61
1	D	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	51	61
1	E	437/444 (98%)	410 (94%)	25 (6%)	2 (0%)	32	37
1	F	434/444 (98%)	414 (95%)	19 (4%)	1 (0%)	51	61
1	G	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	51	61
1	H	435/444 (98%)	389 (89%)	39 (9%)	7 (2%)	11	9
1	I	435/444 (98%)	415 (95%)	18 (4%)	2 (0%)	32	37
1	J	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	51	61
All	All	4349/4440 (98%)	4086 (94%)	238 (6%)	25 (1%)	28	32

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	426	LYS
1	B	429	LYS
1	A	34	ALA

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Mol	Chain	Res	Type
1	A	82	ASP
1	A	117	ARG

### 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	321/356 (90%)	313 (98%)	8 (2%)	53	66
1	B	331/356 (93%)	322 (97%)	9 (3%)	50	63
1	C	336/356 (94%)	327 (97%)	9 (3%)	50	63
1	D	339/356 (95%)	333 (98%)	6 (2%)	64	76
1	E	335/356 (94%)	329 (98%)	6 (2%)	64	76
1	F	338/356 (95%)	329 (97%)	9 (3%)	50	63
1	G	340/356 (96%)	333 (98%)	7 (2%)	59	72
1	H	329/356 (92%)	322 (98%)	7 (2%)	59	72
1	I	336/356 (94%)	331 (98%)	5 (2%)	70	81
1	J	337/356 (95%)	333 (99%)	4 (1%)	75	86
All	All	3342/3560 (94%)	3272 (98%)	70 (2%)	59	72

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	426	LYS
1	F	122	ARG
1	I	268	ARG
1	E	73	LYS
1	E	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	314	HIS

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Mol	Chain	Res	Type
1	F	347	ASN
1	I	410	GLN
1	E	354	GLN
1	F	64	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	A	189	1,3	8,11,12	0.92	0	6,12,14	1.47	1 (16%)
1	KCX	B	189	1,3	8,11,12	0.95	0	6,12,14	1.40	1 (16%)
1	KCX	C	189	1,3	8,11,12	1.06	1 (12%)	6,12,14	1.18	1 (16%)
1	KCX	D	189	1,3	8,11,12	0.99	1 (12%)	6,12,14	1.23	1 (16%)
1	KCX	E	189	1,3	8,11,12	1.06	1 (12%)	6,12,14	1.38	1 (16%)
1	KCX	F	189	1,3	8,11,12	0.94	1 (12%)	6,12,14	1.42	1 (16%)
1	KCX	G	189	1,3	8,11,12	1.02	1 (12%)	6,12,14	1.08	0
1	KCX	H	189	1,3	8,11,12	0.96	0	6,12,14	1.38	1 (16%)
1	KCX	I	189	1,3	8,11,12	1.03	1 (12%)	6,12,14	1.22	1 (16%)
1	KCX	J	189	1,3	8,11,12	0.97	1 (12%)	6,12,14	1.43	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	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	F	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	G	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	H	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	I	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	J	189	1,3	-	0/6/10/12	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	189	KCX	CA-C	2.02	1.52	1.50
1	F	189	KCX	CA-C	2.03	1.52	1.50
1	I	189	KCX	CA-C	2.06	1.53	1.50
1	G	189	KCX	CA-C	2.08	1.53	1.50
1	D	189	KCX	CA-C	2.13	1.53	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	KCX	CE-NZ-CX	-2.93	119.76	123.35
1	F	189	KCX	CE-NZ-CX	-2.86	119.85	123.35
1	B	189	KCX	CE-NZ-CX	-2.82	119.89	123.35
1	E	189	KCX	CE-NZ-CX	-2.71	120.03	123.35
1	J	189	KCX	CE-NZ-CX	-2.71	120.04	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	H	189	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CAP	A	600	3	14,20,20	0.76	0	17,31,31	0.80	0
2	CAP	B	600	3	14,20,20	0.73	0	17,31,31	0.74	0
2	CAP	C	600	3	14,20,20	0.73	0	17,31,31	0.71	0
2	CAP	D	600	3	14,20,20	0.76	0	17,31,31	0.73	0
2	CAP	E	600	3	14,20,20	0.74	0	17,31,31	0.72	0
2	CAP	F	600	3	14,20,20	0.73	0	17,31,31	0.77	0
2	CAP	G	600	3	14,20,20	0.72	0	17,31,31	0.78	0
2	CAP	H	600	3	14,20,20	0.74	0	17,31,31	0.70	0
2	CAP	I	600	3	14,20,20	0.74	0	17,31,31	0.80	0
2	CAP	J	600	3	14,20,20	0.73	0	17,31,31	0.69	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	CAP	A	600	3	-	0/23/29/29	0/0/0/0
2	CAP	B	600	3	-	0/23/29/29	0/0/0/0
2	CAP	C	600	3	-	0/23/29/29	0/0/0/0
2	CAP	D	600	3	-	0/23/29/29	0/0/0/0
2	CAP	E	600	3	-	0/23/29/29	0/0/0/0
2	CAP	F	600	3	-	0/23/29/29	0/0/0/0
2	CAP	G	600	3	-	0/23/29/29	0/0/0/0
2	CAP	H	600	3	-	0/23/29/29	0/0/0/0
2	CAP	I	600	3	-	0/23/29/29	0/0/0/0
2	CAP	J	600	3	-	0/23/29/29	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	CAP	1	0
2	C	600	CAP	1	0
2	E	600	CAP	2	0
2	G	600	CAP	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	435/444 (97%)	0.83	43 (9%) 8 12	28, 41, 56, 60	0
1	B	437/444 (98%)	0.50	35 (8%) 13 19	19, 32, 62, 65	0
1	C	439/444 (98%)	0.27	16 (3%) 43 55	17, 27, 49, 52	0
1	D	436/444 (98%)	0.10	10 (2%) 61 71	16, 24, 35, 42	0
1	E	439/444 (98%)	0.46	42 (9%) 9 13	18, 28, 58, 60	0
1	F	436/444 (98%)	0.32	20 (4%) 33 45	18, 29, 45, 51	0
1	G	436/444 (98%)	0.26	9 (2%) 64 74	18, 31, 44, 48	0
1	H	437/444 (98%)	0.79	50 (11%) 6 9	27, 37, 66, 66	0
1	I	437/444 (98%)	0.22	22 (5%) 30 41	17, 28, 47, 53	0
1	J	437/444 (98%)	0.38	35 (8%) 13 19	16, 25, 59, 60	0
All	All	4369/4440 (98%)	0.41	282 (6%) 20 27	16, 30, 52, 66	0

The worst 5 of 282 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	7.3
1	J	434	ALA	6.5
1	E	441	VAL	6.3
1	E	425	ALA	6.2
1	E	415	ILE	6.2

### 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( $\text{\AA}^2$ )	Q<0.9
1	KCX	E	189	12/13	0.97	0.21	-	22,23,24,24	0
1	KCX	A	189	12/13	0.97	0.22	-	33,33,33,34	0
1	KCX	G	189	12/13	0.98	0.21	-	21,21,22,23	0
1	KCX	C	189	12/13	0.96	0.20	-	24,24,24,24	0
1	KCX	J	189	12/13	0.97	0.23	-	22,23,23,24	0
1	KCX	H	189	12/13	0.96	0.19	-	35,36,37,37	0
1	KCX	F	189	12/13	0.98	0.20	-	22,22,22,22	0
1	KCX	D	189	12/13	0.98	0.20	-	16,18,19,19	0
1	KCX	B	189	12/13	0.97	0.23	-	30,31,32,33	0
1	KCX	I	189	12/13	0.97	0.19	-	24,25,26,26	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( $\text{\AA}^2$ )	Q<0.9
2	CAP	E	600	21/21	0.92	0.24	0.98	31,37,40,41	0
3	MG	E	500	1/1	0.98	0.23	0.53	26,26,26,26	0
2	CAP	J	600	21/21	0.95	0.21	0.18	31,35,38,38	0
2	CAP	H	600	21/21	0.89	0.22	-0.12	41,42,42,43	0
2	CAP	C	600	21/21	0.97	0.18	-0.18	30,31,32,32	0
2	CAP	G	600	21/21	0.98	0.17	-0.52	22,25,26,26	0
2	CAP	D	600	21/21	0.98	0.13	-0.60	16,20,21,21	0
2	CAP	A	600	21/21	0.94	0.17	-1.01	36,38,38,39	0
2	CAP	B	600	21/21	0.97	0.16	-1.19	31,35,36,37	0
2	CAP	F	600	21/21	0.98	0.12	-1.49	22,24,24,25	0
2	CAP	I	600	21/21	0.98	0.10	-1.82	18,21,21,22	0
3	MG	C	500	1/1	0.94	0.16	-2.32	28,28,28,28	0
3	MG	J	500	1/1	0.99	0.13	-2.44	19,19,19,19	0
3	MG	H	500	1/1	0.94	0.16	-3.22	37,37,37,37	0
3	MG	I	500	1/1	0.94	0.10	-3.50	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	500	1/1	0.93	0.10	-4.36	31,31,31,31	0
3	MG	G	500	1/1	0.97	0.09	-5.58	20,20,20,20	0
3	MG	A	500	1/1	0.98	0.13	-5.77	28,28,28,28	0
3	MG	D	500	1/1	0.99	0.08	-7.37	15,15,15,15	0
3	MG	F	500	1/1	0.99	0.10	-8.00	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.