



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:46 AM GMT

PDB ID : 2Y26  
Title : Transmission defective mutant of Grapevine Fanleaf virus  
Authors : Schellenberger, P.; Sauter, C.; Lorber, B.; Bron, P.; Trapani, S.; Bergdoll, M.; Marmonier, A.; Schmitt-Keichinger, C.; Lemaire, O.; Demangeat, G.; Ritzenthaler, C.  
Deposited on : 2010-12-13  
Resolution : 2.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

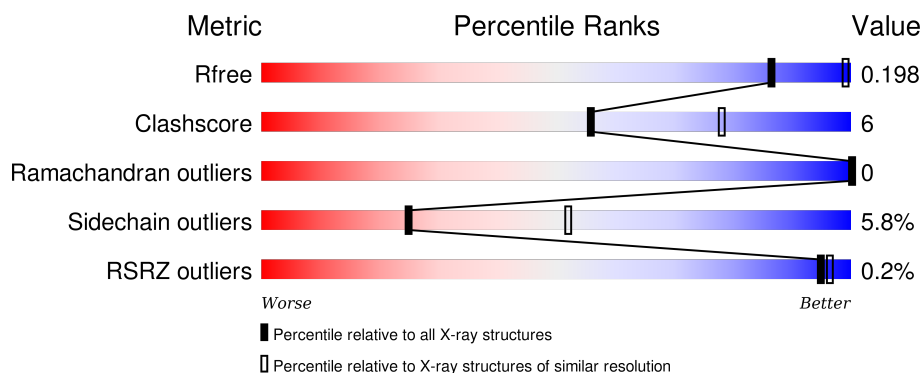
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	504	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	B	504	<div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	504	<div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	D	504	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	E	504	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	504	 85% 13% •
1	G	504	 85% 13% •
1	H	504	 85% 13% •
1	I	504	 85% 13% •
1	J	504	 85% 13% •
1	K	504	 84% 14% •
1	L	504	 85% 14% •
1	M	504	 85% 13% •
1	N	504	 83% 15% •
1	O	504	 85% 13% •
1	P	504	 85% 13% •
1	Q	504	 86% 12% •
1	R	504	 85% 13% •
1	S	504	 84% 14% •
1	T	504	 84% 15% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 79656 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	B	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	C	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	D	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	E	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	F	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	G	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	H	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	I	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	J	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	K	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	L	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	M	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	N	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	O	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	P	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	R	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	S	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			
1	T	504	Total	C	N	O	S	0	0	0
			3955	2557	653	723	22			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ASP	GLY	SEE REMARK 999	UNP P18474
B	297	ASP	GLY	SEE REMARK 999	UNP P18474
C	297	ASP	GLY	SEE REMARK 999	UNP P18474
D	297	ASP	GLY	SEE REMARK 999	UNP P18474
E	297	ASP	GLY	SEE REMARK 999	UNP P18474
F	297	ASP	GLY	SEE REMARK 999	UNP P18474
G	297	ASP	GLY	SEE REMARK 999	UNP P18474
H	297	ASP	GLY	SEE REMARK 999	UNP P18474
I	297	ASP	GLY	SEE REMARK 999	UNP P18474
J	297	ASP	GLY	SEE REMARK 999	UNP P18474
K	297	ASP	GLY	SEE REMARK 999	UNP P18474
L	297	ASP	GLY	SEE REMARK 999	UNP P18474
M	297	ASP	GLY	SEE REMARK 999	UNP P18474
N	297	ASP	GLY	SEE REMARK 999	UNP P18474
O	297	ASP	GLY	SEE REMARK 999	UNP P18474
P	297	ASP	GLY	SEE REMARK 999	UNP P18474
Q	297	ASP	GLY	SEE REMARK 999	UNP P18474
R	297	ASP	GLY	SEE REMARK 999	UNP P18474
S	297	ASP	GLY	SEE REMARK 999	UNP P18474
T	297	ASP	GLY	SEE REMARK 999	UNP P18474

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	30	Total	O	0	0
			30	30		
2	C	27	Total	O	0	0
			27	27		

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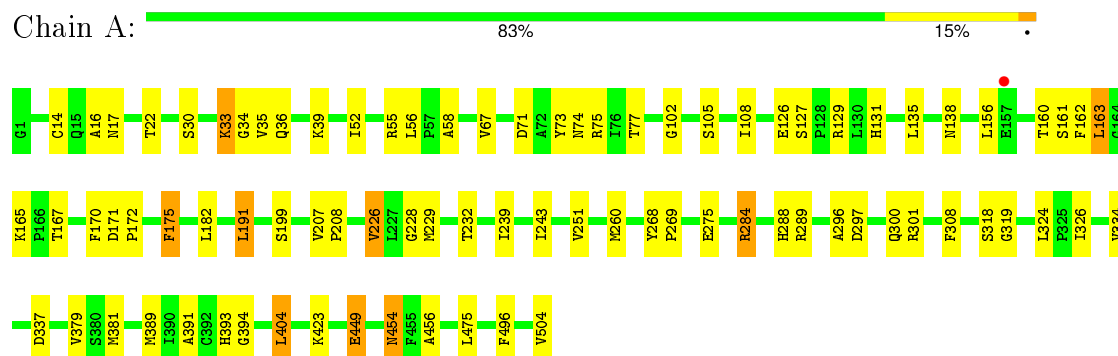
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	28	Total 28	O 28	0	0
2	E	28	Total 28	O 28	0	0
2	F	29	Total 29	O 29	0	0
2	G	26	Total 26	O 26	0	0
2	H	26	Total 26	O 26	0	0
2	I	29	Total 29	O 29	0	0
2	J	27	Total 27	O 27	0	0
2	K	30	Total 30	O 30	0	0
2	L	26	Total 26	O 26	0	0
2	M	29	Total 29	O 29	0	0
2	N	28	Total 28	O 28	0	0
2	O	27	Total 27	O 27	0	0
2	P	28	Total 28	O 28	0	0
2	Q	27	Total 27	O 27	0	0
2	R	27	Total 27	O 27	0	0
2	S	29	Total 29	O 29	0	0
2	T	28	Total 28	O 28	0	0

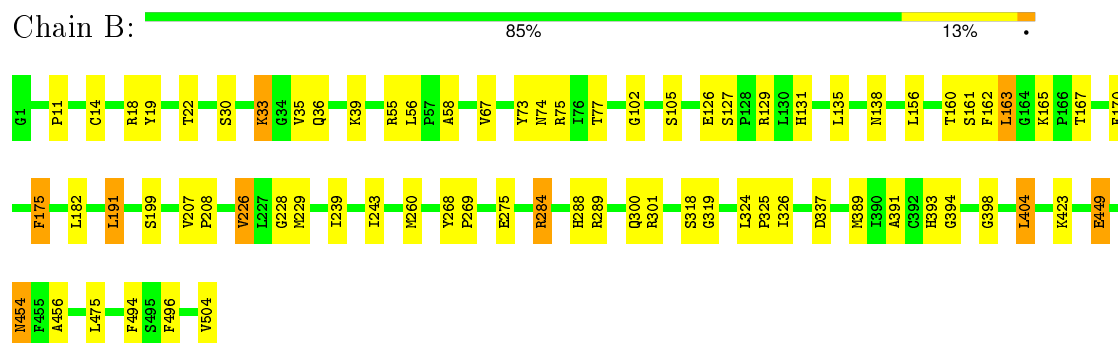
### 3 Residue-property plots

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

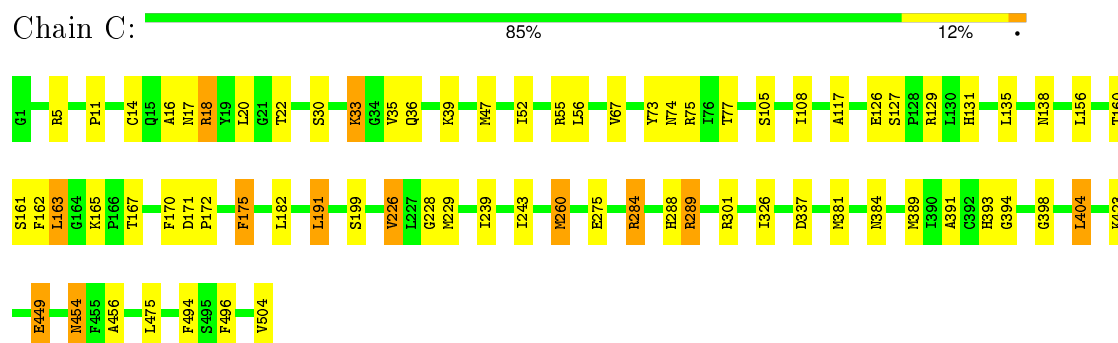
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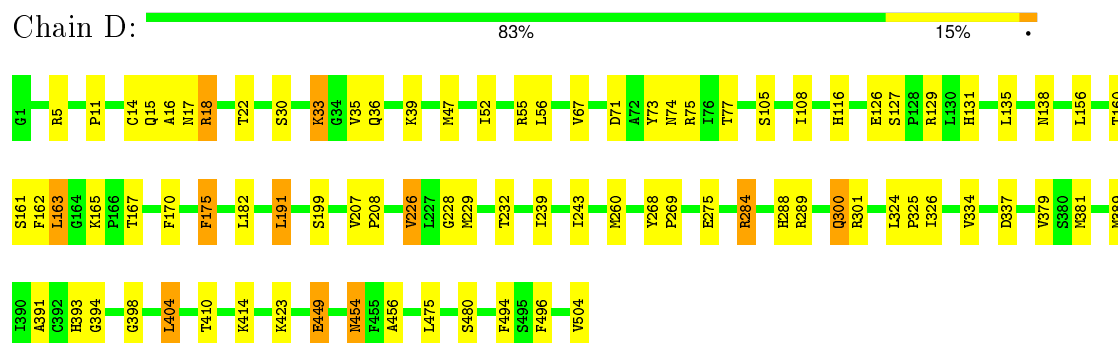
#### • Molecule 1: COAT PROTEIN



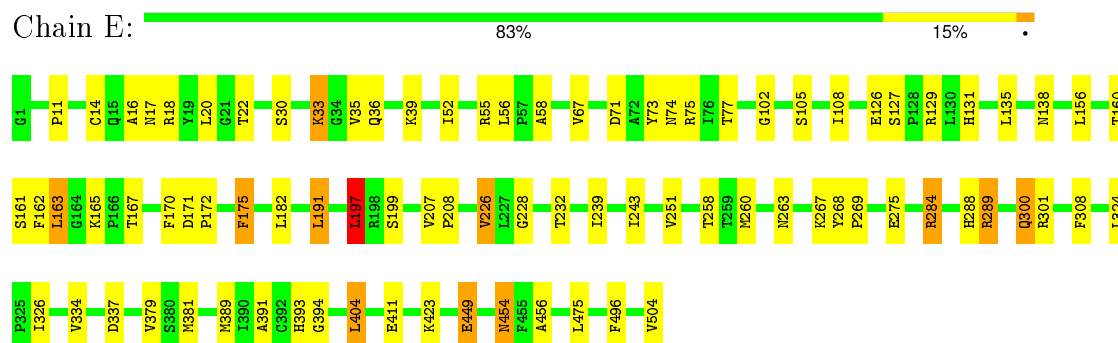
#### • Molecule 1: COAT PROTEIN



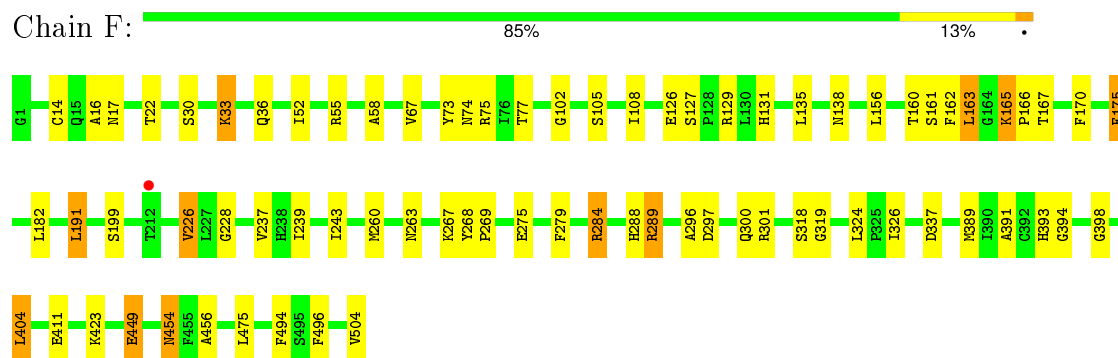
#### • Molecule 1: COAT PROTEIN



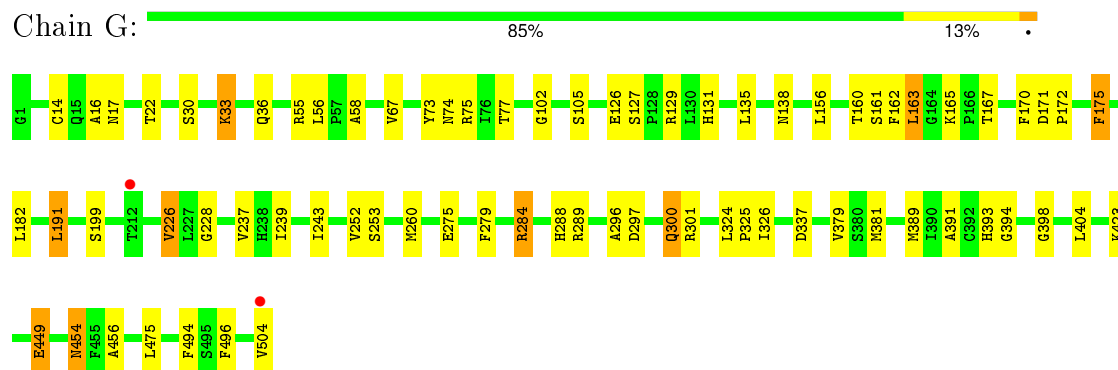
- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN

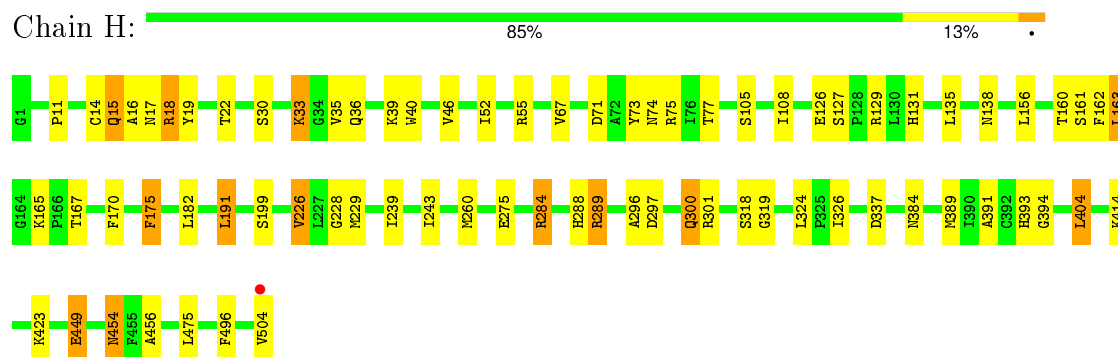


- Molecule 1: COAT PROTEIN

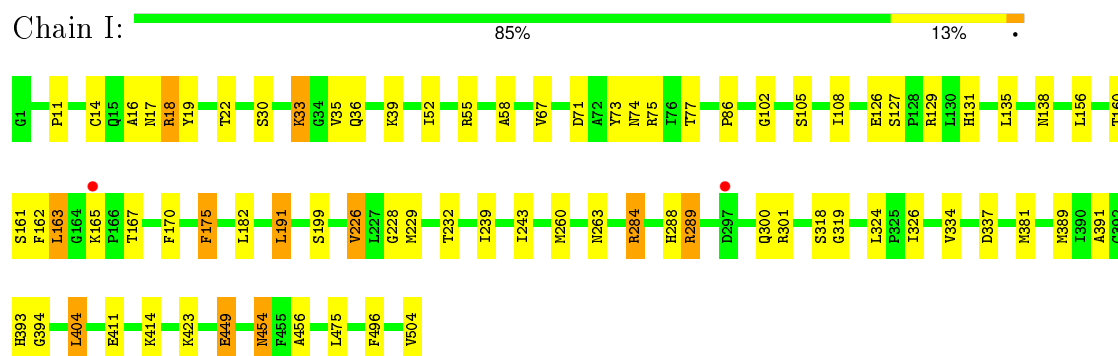


- Molecule 1: COAT PROTEIN

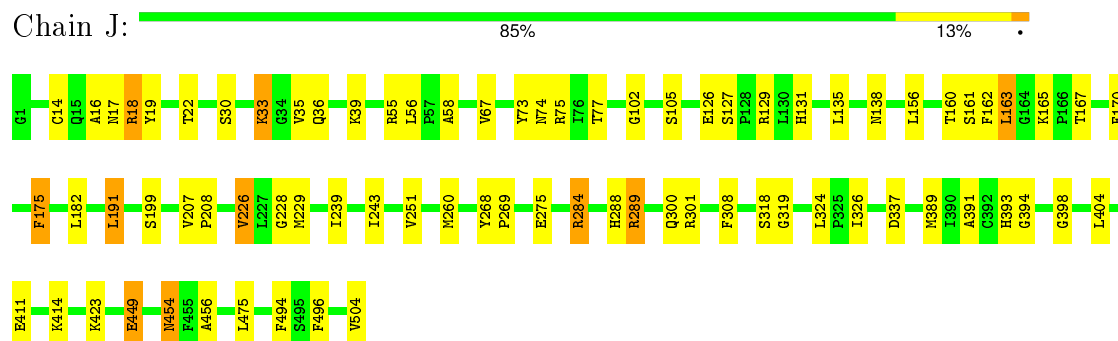




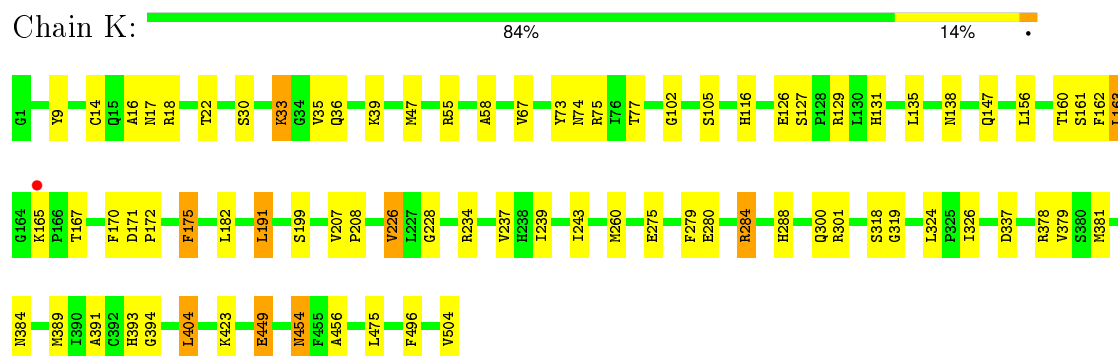
• Molecule 1: COAT PROTEIN



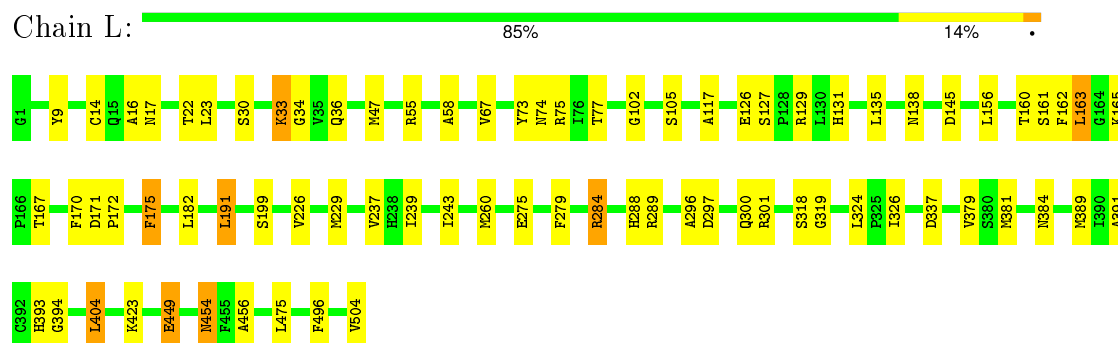
• Molecule 1: COAT PROTEIN



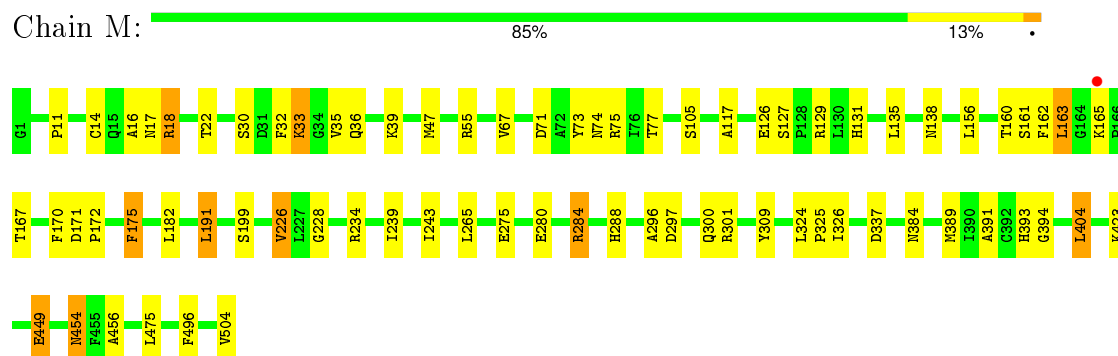
• Molecule 1: COAT PROTEIN



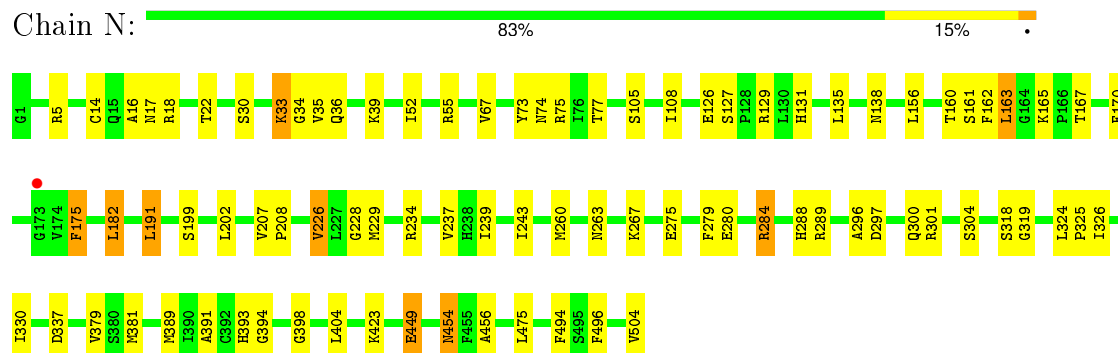
• Molecule 1: COAT PROTEIN



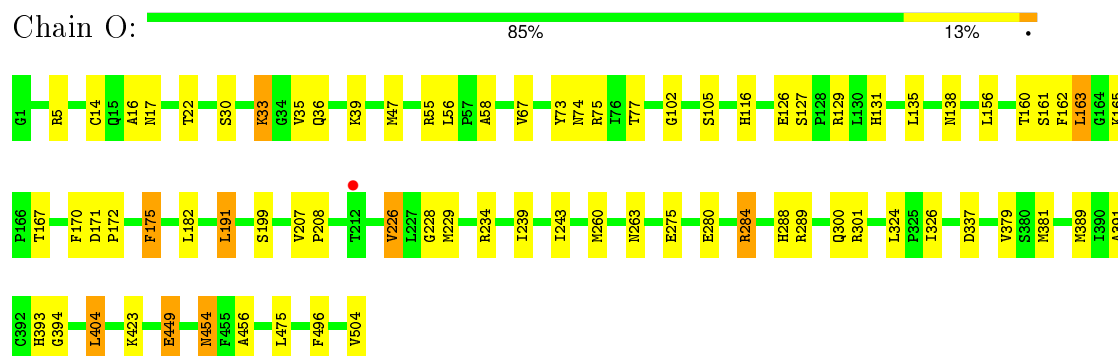
- Molecule 1: COAT PROTEIN



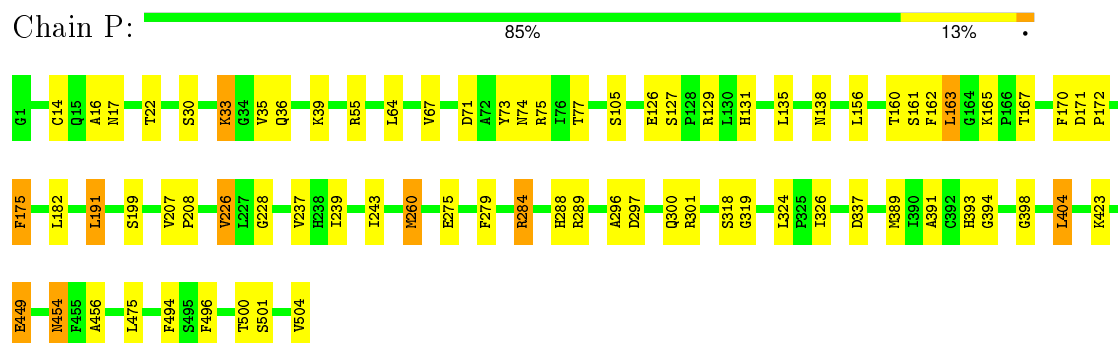
- Molecule 1: COAT PROTEIN



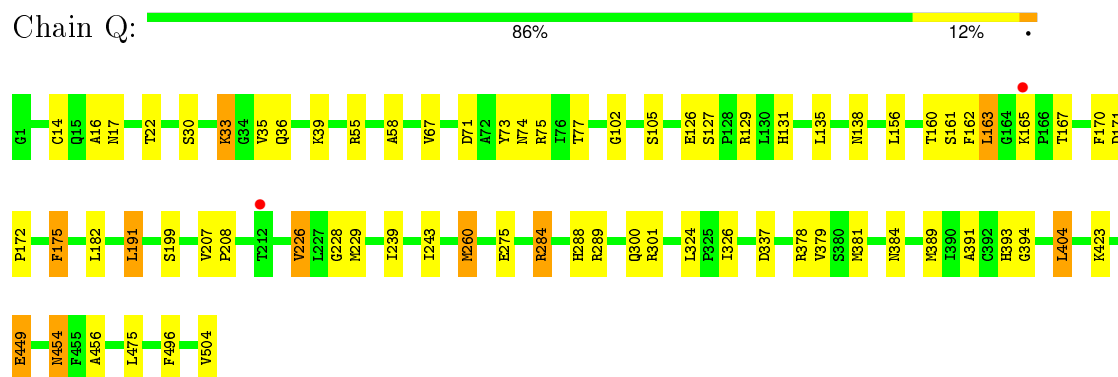
- Molecule 1: COAT PROTEIN



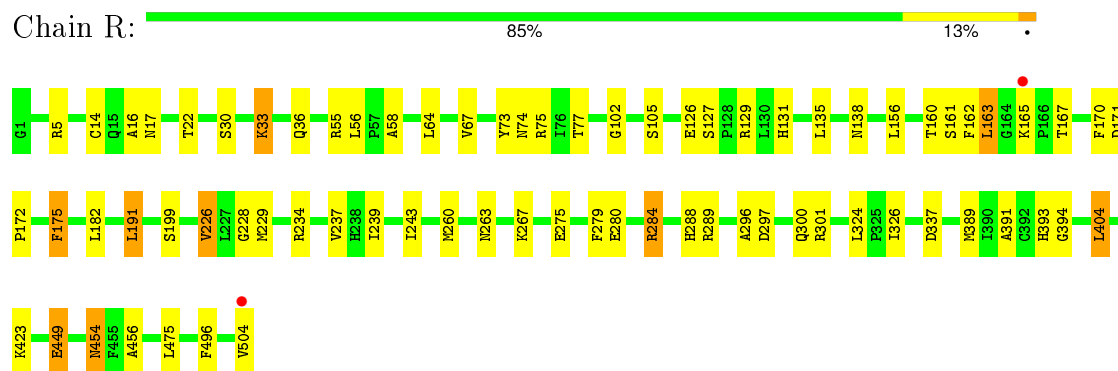
- Molecule 1: COAT PROTEIN



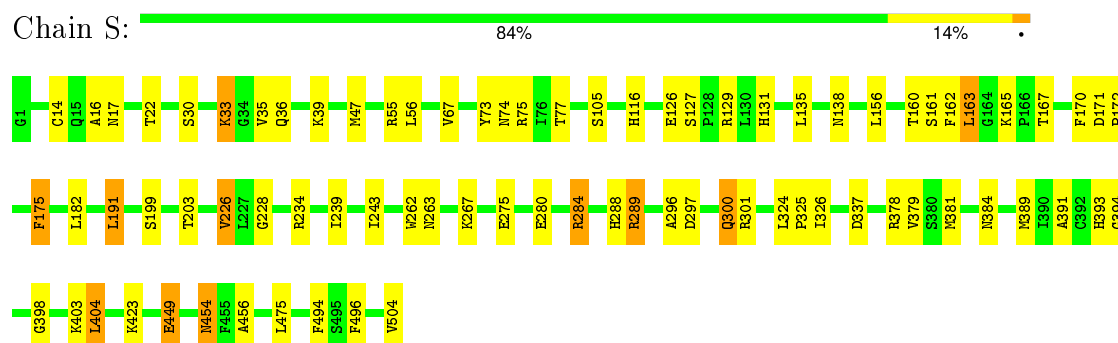
• Molecule 1: COAT PROTEIN



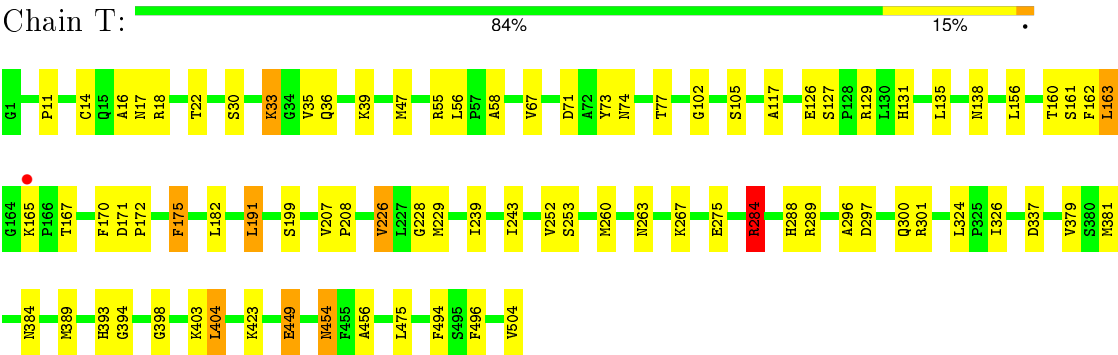
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



● Molecule 1: COAT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	408.00Å 408.00Å 408.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.78 – 2.70 35.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.78-2.70) 98.9 (35.78-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.68Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.193 , 0.210 0.177 , 0.198	Depositor DCC
$R_{free}$ test set	30276 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.0	EDS
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 604441 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	79656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/4062	0.61	1/5523 (0.0%)
1	B	0.47	0/4062	0.61	1/5523 (0.0%)
1	C	0.47	0/4062	0.62	1/5523 (0.0%)
1	D	0.48	0/4062	0.62	1/5523 (0.0%)
1	E	0.48	0/4062	0.62	2/5523 (0.0%)
1	F	0.47	0/4062	0.60	0/5523
1	G	0.47	0/4062	0.61	1/5523 (0.0%)
1	H	0.48	0/4062	0.61	0/5523
1	I	0.49	0/4062	0.62	0/5523
1	J	0.47	0/4062	0.61	1/5523 (0.0%)
1	K	0.47	0/4062	0.61	0/5523
1	L	0.46	0/4062	0.60	0/5523
1	M	0.48	0/4062	0.62	0/5523
1	N	0.47	0/4062	0.61	0/5523
1	O	0.46	0/4062	0.61	1/5523 (0.0%)
1	P	0.48	0/4062	0.61	0/5523
1	Q	0.47	0/4062	0.62	0/5523
1	R	0.48	0/4062	0.62	1/5523 (0.0%)
1	S	0.46	0/4062	0.61	1/5523 (0.0%)
1	T	0.47	0/4062	0.62	2/5523 (0.0%)
All	All	0.47	0/81240	0.61	13/110460 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
All	All	0	40

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	197	LEU	CB-CG-CD2	5.58	120.48	111.00
1	D	56	LEU	CA-CB-CG	5.51	127.98	115.30
1	R	56	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	56	LEU	CA-CB-CG	5.46	127.87	115.30
1	E	56	LEU	CA-CB-CG	5.44	127.81	115.30

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	LYS	Peptide
1	A	55	ARG	Peptide
1	B	33	LYS	Peptide
1	B	55	ARG	Peptide
1	C	33	LYS	Peptide

## 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	3955	0	3910	51	0
1	B	3955	0	3910	46	0
1	C	3955	0	3910	47	0
1	D	3955	0	3910	54	0
1	E	3955	0	3910	57	0
1	F	3955	0	3910	48	0
1	G	3955	0	3910	48	0
1	H	3955	0	3910	50	0
1	I	3955	0	3910	50	0
1	J	3955	0	3910	47	0
1	K	3955	0	3910	50	0
1	L	3955	0	3910	47	0
1	M	3955	0	3910	46	0
1	N	3955	0	3910	55	0
1	O	3955	0	3910	48	0
1	P	3955	0	3910	48	0
1	Q	3955	0	3910	47	0
1	R	3955	0	3910	46	0
1	S	3955	0	3910	50	0
1	T	3955	0	3910	49	0
2	A	27	0	0	1	0
2	B	30	0	0	1	0
2	C	27	0	0	1	0
2	D	28	0	0	1	0
2	E	28	0	0	1	0
2	F	29	0	0	1	0
2	G	26	0	0	0	0
2	H	26	0	0	1	0
2	I	29	0	0	1	0
2	J	27	0	0	1	0
2	K	30	0	0	0	0
2	L	26	0	0	1	0
2	M	29	0	0	0	0
2	N	28	0	0	1	0
2	O	27	0	0	0	0
2	P	28	0	0	0	0
2	Q	27	0	0	0	0
2	R	27	0	0	1	0
2	S	29	0	0	1	0
2	T	28	0	0	0	0
All	All	79656	0	78200	973	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 973 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:454:ASN:HD22	1:G:456:ALA:H	1.28	0.81
1:K:454:ASN:HD22	1:K:456:ALA:H	1.29	0.81
1:G:14:CYS:H	1:G:138:ASN:HD21	1.30	0.80
1:F:191:LEU:HD23	1:F:191:LEU:H	1.46	0.80
1:N:14:CYS:H	1:N:138:ASN:HD21	1.28	0.79

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	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	B	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	C	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	D	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	E	502/504 (100%)	480 (96%)	22 (4%)	0	100	100
1	F	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	G	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	H	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	I	502/504 (100%)	480 (96%)	22 (4%)	0	100	100
1	J	502/504 (100%)	477 (95%)	25 (5%)	0	100	100
1	K	502/504 (100%)	478 (95%)	24 (5%)	0	100	100
1	L	502/504 (100%)	482 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	N	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	O	502/504 (100%)	480 (96%)	22 (4%)	0	100	100
1	P	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	Q	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	R	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	S	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	T	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
All	All	10040/10080 (100%)	9611 (96%)	429 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	B	431/431 (100%)	407 (94%)	24 (6%)	26	54
1	C	431/431 (100%)	405 (94%)	26 (6%)	24	50
1	D	431/431 (100%)	405 (94%)	26 (6%)	24	50
1	E	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	F	431/431 (100%)	407 (94%)	24 (6%)	26	54
1	G	431/431 (100%)	408 (95%)	23 (5%)	28	57
1	H	431/431 (100%)	403 (94%)	28 (6%)	21	46
1	I	431/431 (100%)	405 (94%)	26 (6%)	24	50
1	J	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	K	431/431 (100%)	405 (94%)	26 (6%)	24	50
1	L	431/431 (100%)	405 (94%)	26 (6%)	24	50
1	M	431/431 (100%)	407 (94%)	24 (6%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	O	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	P	431/431 (100%)	407 (94%)	24 (6%)	26	54
1	Q	431/431 (100%)	404 (94%)	27 (6%)	22	48
1	R	431/431 (100%)	407 (94%)	24 (6%)	26	54
1	S	431/431 (100%)	406 (94%)	25 (6%)	25	52
1	T	431/431 (100%)	405 (94%)	26 (6%)	24	50
All	All	8620/8620 (100%)	8116 (94%)	504 (6%)	25	52

5 of 504 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	18	ARG
1	L	161	SER
1	S	226	VAL
1	J	165	LYS
1	K	129	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	15	GLN
1	L	36	GLN
1	S	147	GLN
1	J	74	ASN
1	K	36	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	504/504 (100%)	-0.77	1 (0%) 95 96	26, 36, 60, 83	0
1	B	504/504 (100%)	-0.76	0 100 100	26, 37, 59, 84	0
1	C	504/504 (100%)	-0.77	0 100 100	26, 37, 60, 83	0
1	D	504/504 (100%)	-0.77	0 100 100	26, 38, 60, 84	0
1	E	504/504 (100%)	-0.78	0 100 100	26, 37, 59, 82	0
1	F	504/504 (100%)	-0.83	1 (0%) 95 96	29, 39, 61, 84	0
1	G	504/504 (100%)	-0.82	2 (0%) 93 94	29, 40, 60, 83	0
1	H	504/504 (100%)	-0.77	1 (0%) 95 96	28, 39, 62, 82	0
1	I	504/504 (100%)	-0.74	2 (0%) 93 94	29, 40, 62, 86	0
1	J	504/504 (100%)	-0.74	0 100 100	28, 39, 62, 85	0
1	K	504/504 (100%)	-0.77	1 (0%) 95 96	27, 39, 61, 86	0
1	L	504/504 (100%)	-0.80	0 100 100	27, 38, 59, 81	0
1	M	504/504 (100%)	-0.75	1 (0%) 95 96	29, 38, 60, 86	0
1	N	504/504 (100%)	-0.74	1 (0%) 95 96	28, 38, 59, 83	0
1	O	504/504 (100%)	-0.81	1 (0%) 95 96	28, 38, 60, 83	0
1	P	504/504 (100%)	-0.74	0 100 100	28, 38, 60, 81	0
1	Q	504/504 (100%)	-0.75	2 (0%) 93 94	27, 38, 60, 86	0
1	R	504/504 (100%)	-0.77	2 (0%) 93 94	27, 38, 61, 83	0
1	S	504/504 (100%)	-0.80	0 100 100	28, 38, 59, 84	0
1	T	504/504 (100%)	-0.80	1 (0%) 95 96	28, 38, 60, 84	0
All	All	10080/10080 (100%)	-0.77	16 (0%) 95 96	26, 38, 60, 86	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	165	LYS	3.3
1	N	173	GLY	3.2
1	O	212	THR	3.0
1	M	165	LYS	2.9
1	I	165	LYS	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.