



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 4HHH  
Title : Structure of Pisum sativum Rubisco  
Authors : Loewen, P.C.; Didychuk, A.L.; Switala, J.; Loewen, M.C.  
Deposited on : 2012-10-09  
Resolution : 2.20 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

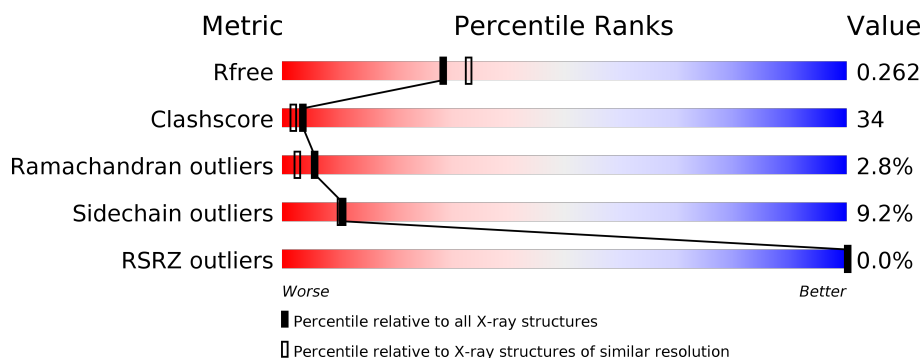
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	475	
1	B	475	
1	C	475	
1	D	475	
2	S	123	
2	T	123	

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Mol	Chain	Length	Quality of chain
2	U	123	<div><div></div><div>41%45%14%</div></div>
2	V	123	<div>%<div><div></div><div>43%44%12%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

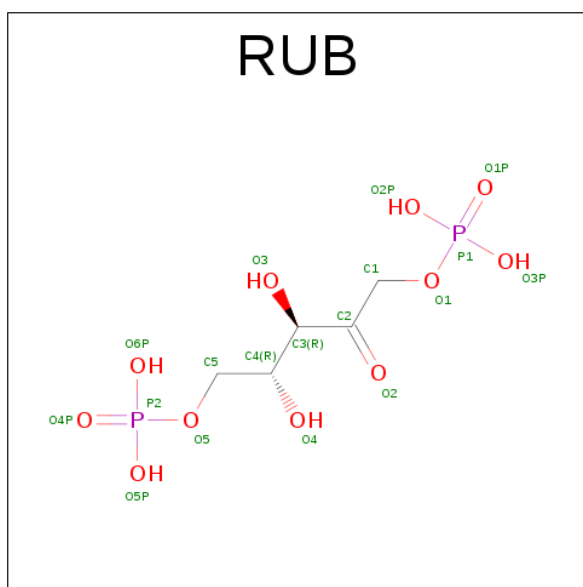
- Molecule 1 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	11	0
			3648	2332	634	664	18			
1	B	458	Total	C	N	O	S	0	13	0
			3653	2340	635	660	18			
1	C	458	Total	C	N	O	S	0	12	0
			3662	2338	644	662	18			
1	D	458	Total	C	N	O	S	0	9	0
			3647	2323	643	663	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	2	0
			1049	694	172	178	5			
2	T	123	Total	C	N	O	S	0	3	0
			1056	698	175	178	5			
2	U	123	Total	C	N	O	S	0	2	0
			1047	690	172	180	5			
2	V	123	Total	C	N	O	S	0	3	0
			1057	697	175	180	5			

- Molecule 3 is SUGAR (RIBULOSE-1,5-DIPHOSPHATE) (three-letter code: RUB) (formula:  $C_5H_{12}O_{11}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			18	5	11	2		
3	B	1	Total	C	O	P	0	0
			18	5	11	2		
3	C	1	Total	C	O	P	0	0
			18	5	11	2		
3	D	1	Total	C	O	P	0	0
			18	5	11	2		

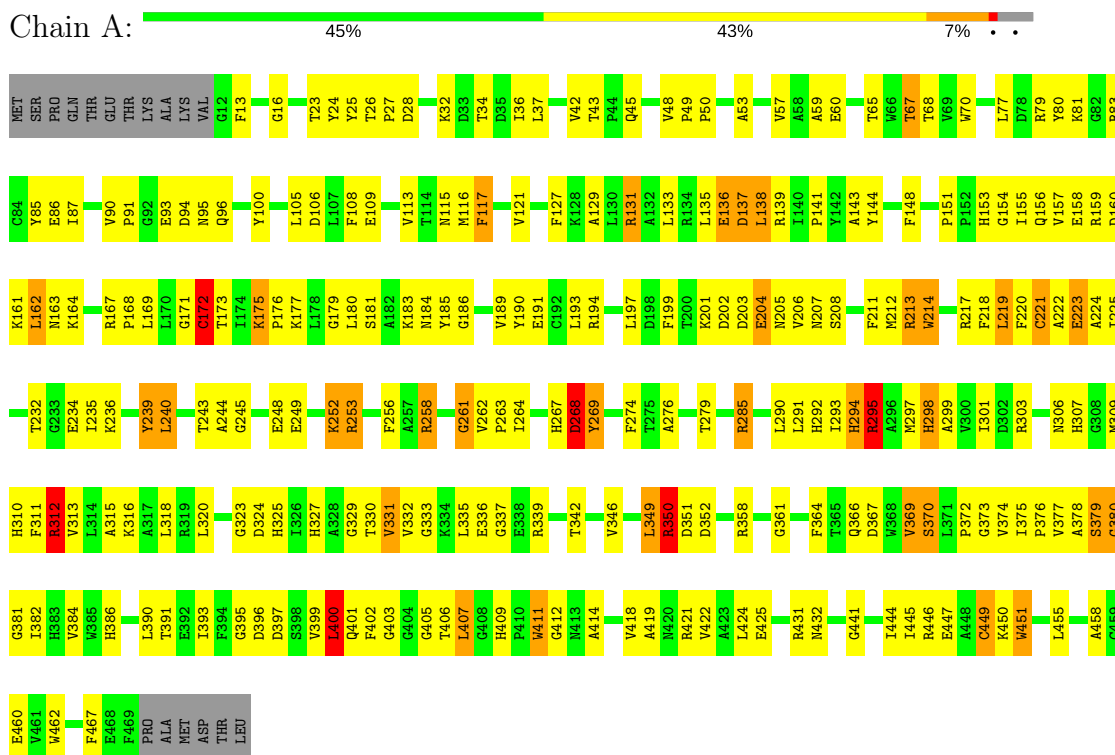
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	175	Total	O	0	0
			175	175		
4	C	137	Total	O	0	0
			137	137		
4	D	147	Total	O	0	0
			147	147		
4	S	49	Total	O	0	0
			49	49		
4	T	50	Total	O	0	0
			50	50		
4	U	30	Total	O	0	0
			30	30		
4	V	40	Total	O	0	0
			40	40		

### 3 Residue-property plots

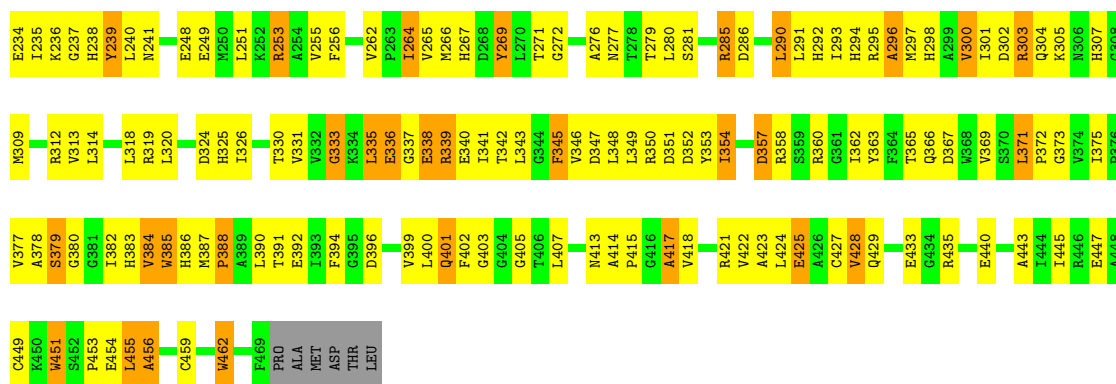
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 large chain



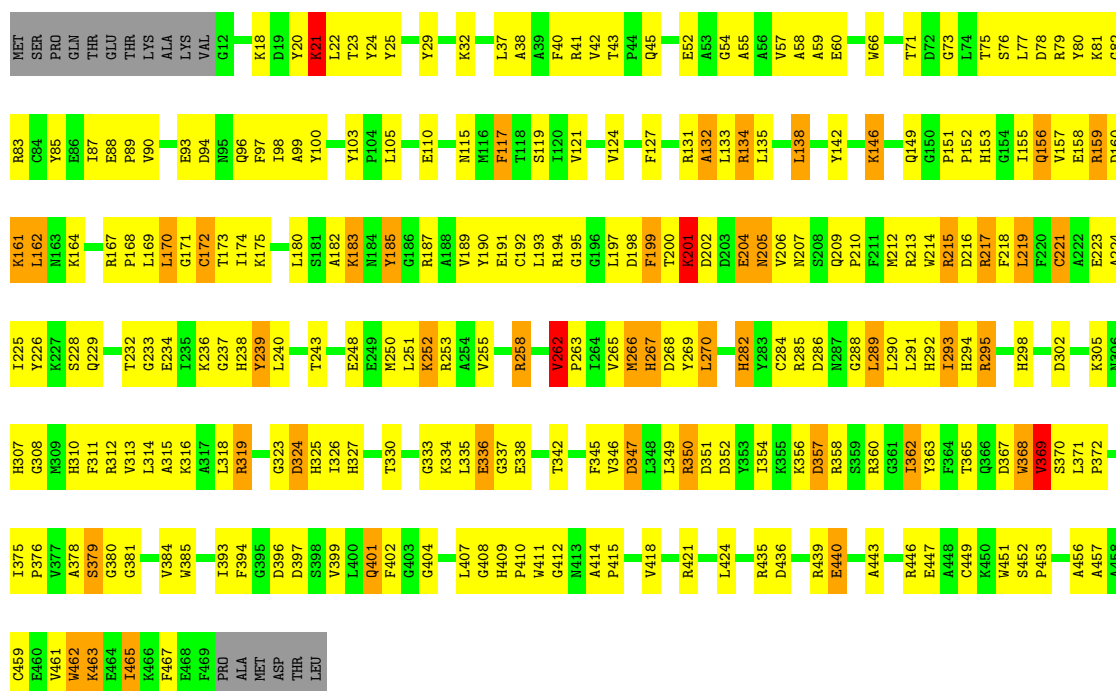
- Molecule 1: Ribulose biphosphate carboxylase large chain

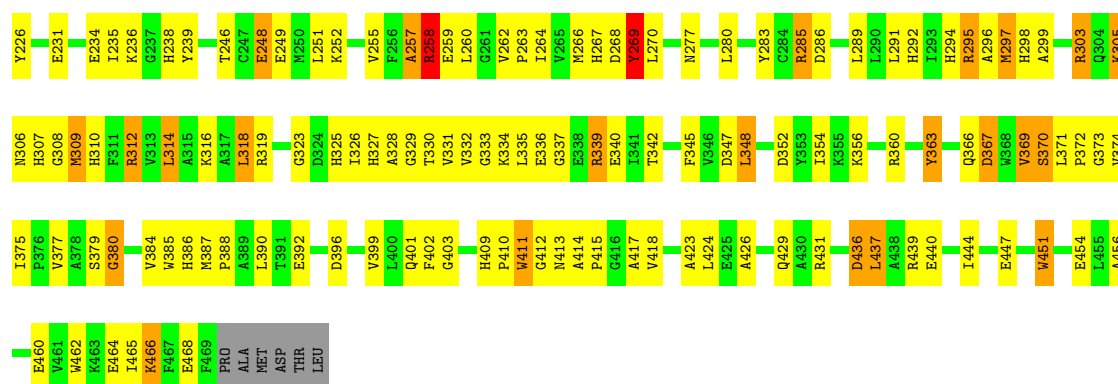




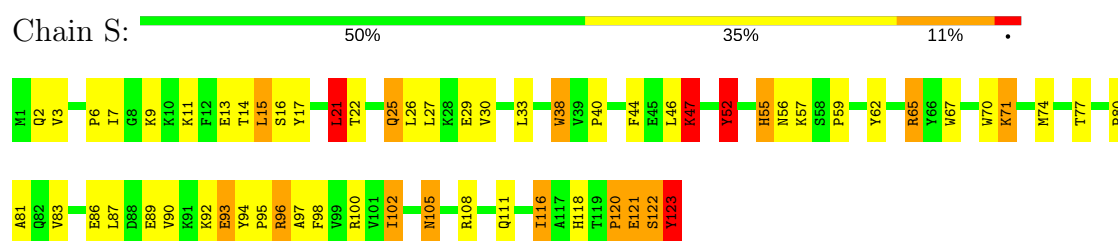
• Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C: 43% 44% 9% . .

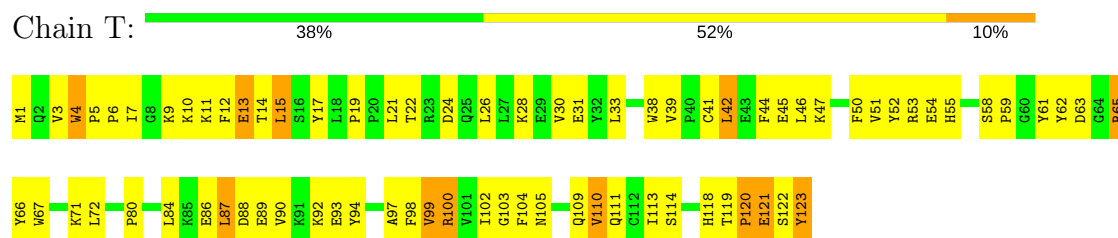




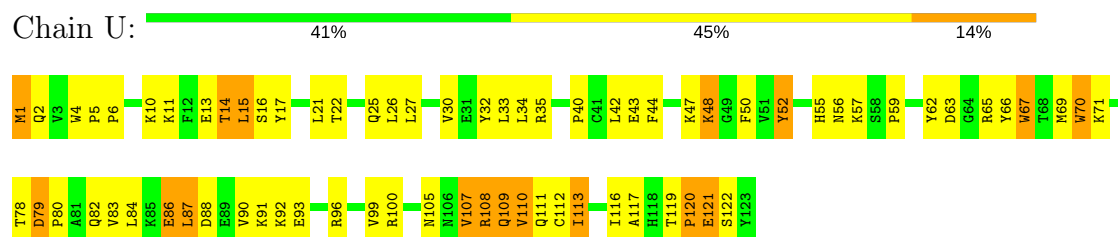
• Molecule 2: Ribulose biphosphate carboxylase small chain



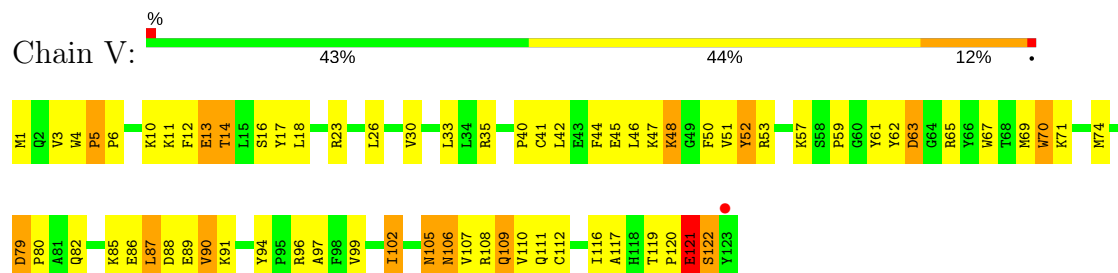
• Molecule 2: Ribulose biphosphate carboxylase small chain



• Molecule 2: Ribulose biphosphate carboxylase small chain



• Molecule 2: Ribulose biphosphate carboxylase small chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.79Å 109.95Å 201.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.95 – 2.20 48.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (109.95-2.20) 93.1 (48.20-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.22	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.197 , 0.279 0.198 , 0.262	Depositor DCC
$R_{free}$ test set	5831 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.4	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 3.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.349 for k,h,-l	Xtriage
Reported twinning fraction	0.580 for H, K, L 0.420 for K, H, -L	Depositor
Outliers	0 of 116024 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	19680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: RUB

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	1.15	9/3765 (0.2%)	1.35	33/5104 (0.6%)
1	B	1.15	4/3783 (0.1%)	1.35	31/5128 (0.6%)
1	C	1.01	6/3790 (0.2%)	1.19	24/5135 (0.5%)
1	D	1.03	8/3758 (0.2%)	1.27	25/5090 (0.5%)
2	S	0.95	3/1089 (0.3%)	1.07	3/1474 (0.2%)
2	T	0.94	1/1099 (0.1%)	1.02	1/1487 (0.1%)
2	U	0.81	3/1087 (0.3%)	0.90	0/1472
2	V	0.84	2/1100 (0.2%)	0.94	3/1489 (0.2%)
All	All	1.04	36/19471 (0.2%)	1.23	120/26379 (0.5%)

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	1
1	C	0	3
2	S	0	1
2	V	0	1
All	All	0	6

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TRP	NE1-CE2	-6.74	1.28	1.37
1	A	373	GLY	N-CA	6.64	1.56	1.46
1	C	204	GLU	CD-OE2	6.45	1.32	1.25
1	D	70	TRP	CD2-CE2	6.11	1.48	1.41
1	D	411	TRP	CD2-CE2	6.07	1.48	1.41

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	D	367	ASP	CB-CG-OD2	9.96	127.27	118.30
1	D	295	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	253	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	160	ASP	CB-CG-OD2	8.97	126.38	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	PHE	Peptide
1	C	195	GLY	Peptide
1	C	199	PHE	Peptide
1	C	93	GLU	Peptide
2	S	47	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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	3648	0	3615	263	2
1	B	3653	0	3642	270	1
1	C	3662	0	3632	268	1
1	D	3647	0	3601	248	3
2	S	1049	0	1065	75	1
2	T	1056	0	1076	83	1
2	U	1047	0	1057	75	1
2	V	1057	0	1071	83	0
3	A	18	0	8	4	0
3	B	18	0	8	4	0
3	C	18	0	8	4	0
3	D	18	0	8	1	0
4	A	161	0	0	28	1
4	B	175	0	0	31	1
4	C	137	0	0	29	1
4	D	147	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	49	0	0	8	0
4	T	50	0	0	3	0
4	U	30	0	0	3	0
4	V	40	0	0	6	0
All	All	19680	0	18791	1296	7

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 34.

The worst 5 of 1296 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:C:201:LYS:NZ	1:C:294:HIS:NE2	1.70	1.35
1:C:201:LYS:HE3	1:C:202:ASP:O	1.40	1.16
1:D:201:LYS:NZ	1:D:294:HIS:NE2	1.98	1.11
1:A:60:GLU:HG3	1:A:127:PHE:HZ	1.04	1.09
1:A:409:HIS:HD2	1:A:458:ALA:HB2	1.16	1.08

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:105:ASN:O	4:A:727:HOH:O[2_555]	1.92	0.28
1:D:207:ASN:ND2	4:C:615:HOH:O[2_555]	1.94	0.26
1:D:75:THR:OG1	2:T:109:GLN:NE2[2_555]	2.00	0.20
1:A:106:ASP:OD2	1:A:370[B]:SER:OG[2_555]	2.05	0.15
1:A:65:THR:CG2	4:B:728:HOH:O[2_555]	2.07	0.13

## 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	467/475 (98%)	405 (87%)	51 (11%)	11 (2%)	7	4
1	B	469/475 (99%)	404 (86%)	48 (10%)	17 (4%)	4	1
1	C	468/475 (98%)	411 (88%)	47 (10%)	10 (2%)	8	5
1	D	465/475 (98%)	408 (88%)	47 (10%)	10 (2%)	8	4
2	S	123/123 (100%)	105 (85%)	12 (10%)	6 (5%)	2	1
2	T	124/123 (101%)	109 (88%)	12 (10%)	3 (2%)	7	4
2	U	123/123 (100%)	97 (79%)	20 (16%)	6 (5%)	2	1
2	V	124/123 (101%)	111 (90%)	9 (7%)	4 (3%)	5	2
All	All	2363/2392 (99%)	2050 (87%)	246 (10%)	67 (3%)	6	3

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	SER
1	B	212	MET
1	C	21	LYS
2	S	120	PRO
2	T	120	PRO

### 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	381/385 (99%)	353 (93%)	28 (7%)	16	17
1	B	383/385 (100%)	348 (91%)	35 (9%)	11	11
1	C	382/385 (99%)	347 (91%)	35 (9%)	11	10
1	D	379/385 (98%)	341 (90%)	38 (10%)	9	8
2	S	115/113 (102%)	101 (88%)	14 (12%)	6	5
2	T	116/113 (103%)	104 (90%)	12 (10%)	8	7
2	U	115/113 (102%)	98 (85%)	17 (15%)	3	2
2	V	116/113 (103%)	103 (89%)	13 (11%)	7	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1987/1992 (100%)	1795 (90%)	192 (10%)	<b>11</b> <b>9</b>

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	293	ILE
1	D	131	ARG
2	U	113	ILE
1	C	365[B]	THR
1	C	465	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	GLN
1	D	30	GLN
2	U	111	GLN
1	C	267	HIS
1	D	96	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

4 ligands 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
3	RUB	A	501	-	16,17,17	1.17	2 (12%)	18,25,25	1.94	7 (38%)
3	RUB	B	501	-	16,17,17	1.74	4 (25%)	18,25,25	2.88	7 (38%)
3	RUB	C	501	-	16,17,17	0.74	0	18,25,25	2.47	10 (55%)
3	RUB	D	501	-	16,17,17	0.96	0	18,25,25	1.82	6 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RUB	A	501	-	-	0/20/20/20	0/0/0/0
3	RUB	B	501	-	-	0/20/20/20	0/0/0/0
3	RUB	C	501	-	-	0/20/20/20	0/0/0/0
3	RUB	D	501	-	-	0/20/20/20	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	RUB	C5-C4	2.24	1.55	1.51
3	B	501	RUB	O3-C3	2.32	1.47	1.42
3	A	501	RUB	O3-C3	2.51	1.47	1.42
3	B	501	RUB	P2-O5	2.73	1.69	1.60
3	B	501	RUB	O2-C2	3.50	1.27	1.21

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	RUB	C5-C4-C3	-7.87	99.01	111.83
3	B	501	RUB	O5P-P2-O5	-3.96	96.20	106.73
3	D	501	RUB	O5-P2-O4P	-3.74	95.98	106.47
3	C	501	RUB	O5P-P2-O5	-3.49	97.46	106.73
3	C	501	RUB	O4-C4-C5	-3.14	103.01	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	RUB	4	0
3	B	501	RUB	4	0
3	C	501	RUB	4	0
3	D	501	RUB	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	458/475 (96%)	-0.96	0	100	100	2, 2, 20, 43	0
1	B	458/475 (96%)	-0.97	0	100	100	2, 2, 23, 46	0
1	C	458/475 (96%)	-0.86	0	100	100	2, 9, 28, 34	0
1	D	458/475 (96%)	-0.89	0	100	100	2, 10, 30, 37	0
2	S	123/123 (100%)	-0.80	0	100	100	2, 15, 24, 34	0
2	T	123/123 (100%)	-0.80	0	100	100	2, 14, 27, 52	0
2	U	123/123 (100%)	-0.61	0	100	100	7, 23, 37, 46	0
2	V	123/123 (100%)	-0.61	1 (0%)	86	85	5, 19, 31, 58	0
All	All	2324/2392 (97%)	-0.88	1 (0%)	100	100	2, 8, 29, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	123	TYR	3.2

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	RUB	B	501	18/18	0.98	0.09	0.79	2,2,2,2	0
3	RUB	A	501	18/18	0.97	0.08	-0.20	6,10,12,12	0
3	RUB	C	501	18/18	0.99	0.07	-0.89	8,11,16,17	0
3	RUB	D	501	18/18	0.98	0.07	-1.39	8,14,18,19	0

## 6.5 Other polymers

There are no such residues in this entry.