



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:52 pm BST

PDB ID : 1V6O  
Title : Peanut lectin complexed with 10mer peptide (PVRIWSSATG)  
Authors : Kundhavai Natchiar, S.; Arockia Jeyaprakash, A.; Ramya, T.N.C.; Thomas, C.J.; Suguna, K.; Surolia, A.; Vijayan, M.  
Deposited on : 2003-12-02  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

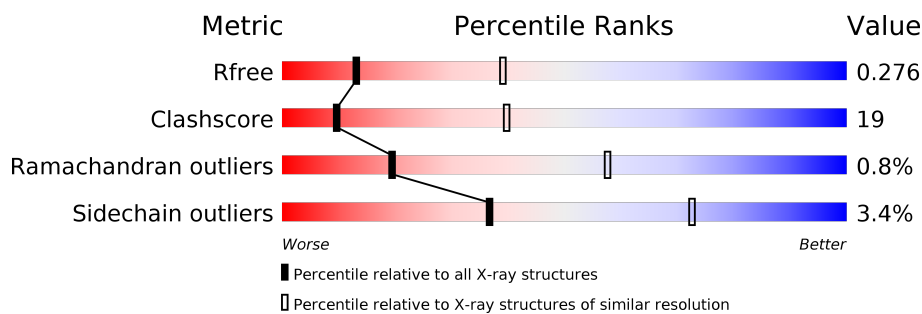
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	232	63% 34% .
1	B	232	63% 34% .
1	C	232	70% 28% .
1	D	232	61% 36% .
1	E	232	66% 32% .
1	F	232	71% 27% .
1	G	232	69% 29% .

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Mol	Chain	Length	Quality of chain
1	H	232	 A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment on the left representing 69% and a yellow segment on the right representing 30%. A small red dot is at the far right end of the bar. <div>69%30%.</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14228 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 Galactose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	B	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	C	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	D	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	E	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	F	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	G	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			
1	H	232	Total	C	N	O	S	0	0	0
			1744	1102	287	353	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Mn 1	0	0
3	D	1	Total 1	Mn 1	0	0
3	E	1	Total 1	Mn 1	0	0
3	H	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0
3	F	1	Total 1	Mn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	B	34	Total 34	O 34	0	0
4	C	29	Total 29	O 29	0	0
4	D	17	Total 17	O 17	0	0
4	E	51	Total 51	O 51	0	0
4	F	35	Total 35	O 35	0	0
4	G	28	Total 28	O 28	0	0

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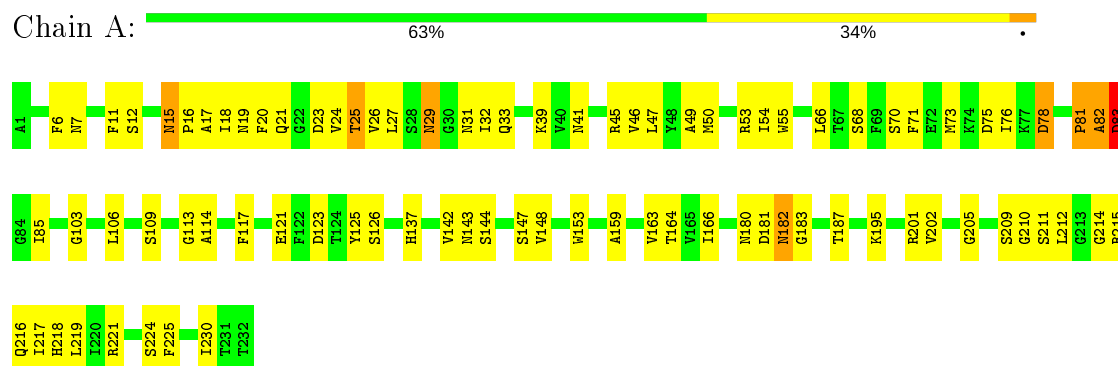
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	26	Total	O	0	0
			26	26		

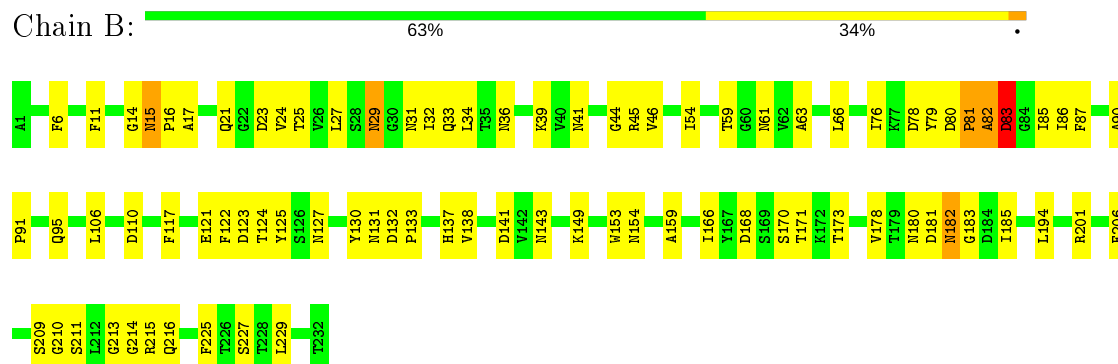
### 3 Residue-property plots

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. 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. 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.

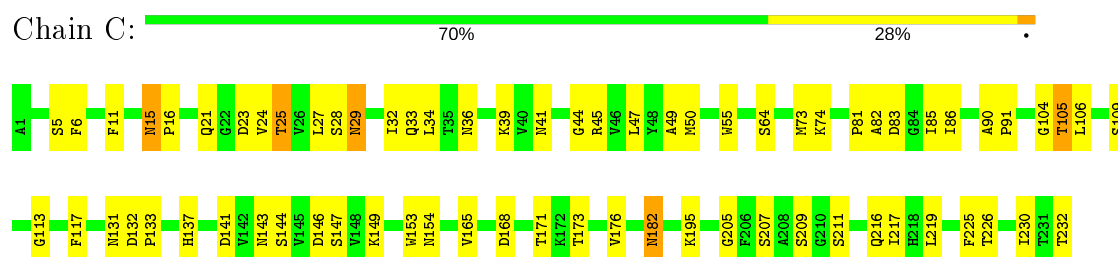
#### • Molecule 1: Galactose-binding lectin



#### • Molecule 1: Galactose-binding lectin

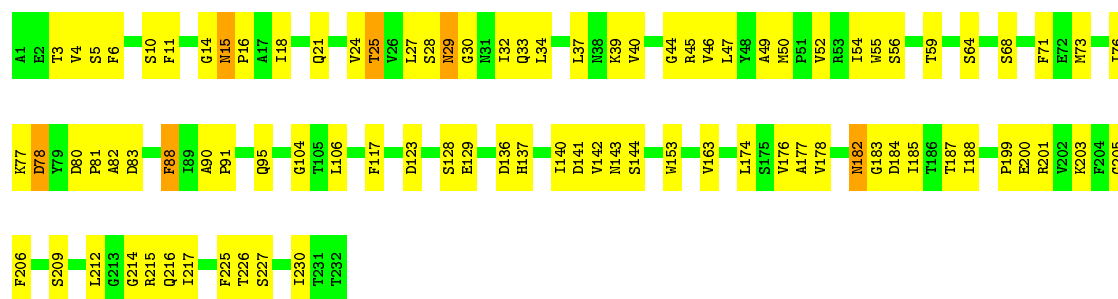


#### • Molecule 1: Galactose-binding lectin



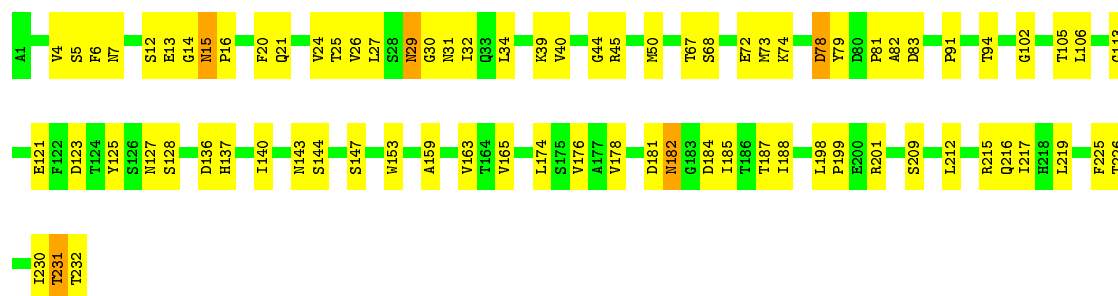
#### • Molecule 1: Galactose-binding lectin

Chain D:  61% 36%



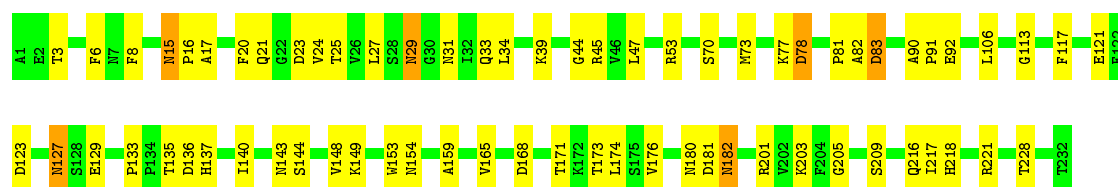
• Molecule 1: Galactose-binding lectin

Chain E:  66% 32%



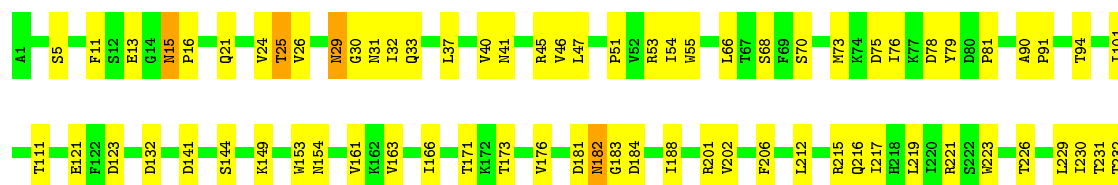
• Molecule 1: Galactose-binding lectin

Chain F:  71% 27%



• Molecule 1: Galactose-binding lectin

Chain G:  69% 29%



• Molecule 1: Galactose-binding lectin

Chain H:  69% 30%



A1	E2	T3	F6	F11	S12	E13	G14	M15	P16	A17	F20	Q21	G22	D23	V24	T25	S28	N29	I32	Q33	L34	L37	N38	K39	V40	M41	G44	R45	V46	I54	W55	T67	S68	P69	S70	M73	K74	D75	I76	K77	D78	Y79	P81	A82	D83	G84	I85	I86
A90	P91	I101	S109	D110	T111	K112	G113	A114	E129	Y130	P133	H137	W153	N154	V161	K162	V163	T164	V165	V176	M182	G183	D184	I188	V191	F206	S207	G210	S211	L212	R215	Q216	I217	H218	W223	S224	F225	T228	L229	I230	T231	T232						

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.13Å 125.80Å 84.74Å 90.00° 116.19° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 9.96 – 2.98	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-3.00) 88.2 (9.96-2.98)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.174 , 0.239 0.224 , 0.276	Depositor DCC
$R_{free}$ test set	2521 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: CA, MN

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	0.38	0/1780	0.73	2/2426 (0.1%)
1	B	0.38	0/1780	0.71	2/2426 (0.1%)
1	C	0.37	0/1780	0.65	0/2426
1	D	0.35	0/1780	0.64	0/2426
1	E	0.39	0/1780	0.68	0/2426
1	F	0.37	0/1780	0.69	2/2426 (0.1%)
1	G	0.37	0/1780	0.67	0/2426
1	H	0.36	0/1780	0.66	0/2426
All	All	0.37	0/14240	0.68	6/19408 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASP	N-CA-C	-9.43	85.54	111.00
1	B	83	ASP	N-CA-C	-7.42	90.96	111.00
1	B	82	ALA	N-CA-C	6.14	127.57	111.00
1	A	82	ALA	N-CA-C	5.72	126.44	111.00
1	F	78	ASP	N-CA-C	-5.36	96.52	111.00

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	1744	0	1699	83	0
1	B	1744	0	1699	90	0
1	C	1744	0	1699	61	0
1	D	1744	0	1699	74	0
1	E	1744	0	1699	67	0
1	F	1744	0	1699	68	0
1	G	1744	0	1699	66	0
1	H	1744	0	1699	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	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
4	A	40	0	0	3	0
4	B	34	0	0	2	0
4	C	29	0	0	0	0
4	D	17	0	0	1	0
4	E	51	0	0	1	0
4	F	35	0	0	2	0
4	G	28	0	0	2	0
4	H	26	0	0	1	0
All	All	14228	0	13592	535	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 19.

The worst 5 of 535 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:B:83:ASP:HB3	1:B:125:TYR:HB3	1.36	1.05
1:A:21:GLN:NE2	1:A:45:ARG:HE	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:GLN:HE22	1:F:45:ARG:HH21	1.14	0.94
1:E:81:PRO:HB3	1:E:216:GLN:NE2	1.84	0.92
1:H:21:GLN:HE22	1:H:45:ARG:HH21	1.12	0.92

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	230/232 (99%)	208 (90%)	19 (8%)	3 (1%)	12	45
1	B	230/232 (99%)	209 (91%)	20 (9%)	1 (0%)	34	72
1	C	230/232 (99%)	213 (93%)	14 (6%)	3 (1%)	12	45
1	D	230/232 (99%)	210 (91%)	19 (8%)	1 (0%)	34	72
1	E	230/232 (99%)	213 (93%)	15 (6%)	2 (1%)	17	55
1	F	230/232 (99%)	211 (92%)	18 (8%)	1 (0%)	34	72
1	G	230/232 (99%)	210 (91%)	20 (9%)	0	100	100
1	H	230/232 (99%)	208 (90%)	18 (8%)	4 (2%)	9	39
All	All	1840/1856 (99%)	1682 (91%)	143 (8%)	15 (1%)	19	57

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	B	81	PRO
1	C	147	SER
1	D	128	SER
1	F	23	ASP

### 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	197/197 (100%)	189 (96%)	8 (4%)	30	67
1	B	197/197 (100%)	189 (96%)	8 (4%)	30	67
1	C	197/197 (100%)	191 (97%)	6 (3%)	41	75
1	D	197/197 (100%)	191 (97%)	6 (3%)	41	75
1	E	197/197 (100%)	190 (96%)	7 (4%)	35	70
1	F	197/197 (100%)	190 (96%)	7 (4%)	35	70
1	G	197/197 (100%)	191 (97%)	6 (3%)	41	75
1	H	197/197 (100%)	192 (98%)	5 (2%)	47	79
All	All	1576/1576 (100%)	1523 (97%)	53 (3%)	37	72

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	THR
1	E	15	ASN
1	H	15	ASN
1	D	29	ASN
1	D	88	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	61	ASN
1	E	31	ASN
1	H	41	ASN
1	D	95	GLN
1	D	218	HIS

### 5.3.3 RNA ⓘ

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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.