



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:48 PM GMT

PDB ID : 1I6H  
Title : RNA POLYMERASE II ELONGATION COMPLEX  
Authors : Gnatt, A.L.; Cramer, P.; Kornberg, R.D.  
Deposited on : 2001-03-02  
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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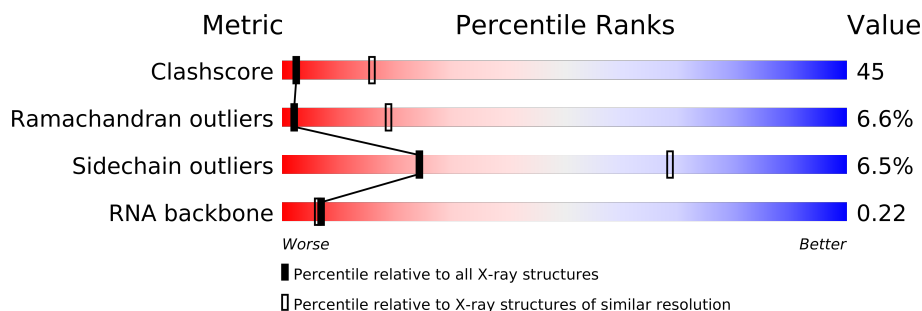
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	13	
2	R	9	
3	A	1733	
4	B	1224	
5	C	318	
6	E	215	
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28430 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(P\*AP\*AP\*AP\*TP\*GP\*CP\*CP\*TP\*GP\*GP\*TP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			

- Molecule 2 is a RNA chain called 5'-R(P\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	9	Total	C	N	O	P	0	0	0
			196	87	39	61	9			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	C	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		
13	L	1	Total	Zn	0	0
			1	1		

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	R	1	Total	Mg	0	0
			1	1		

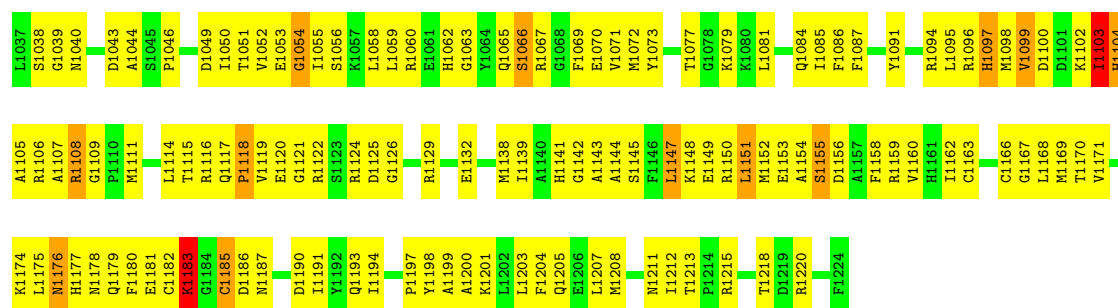




Chain B:

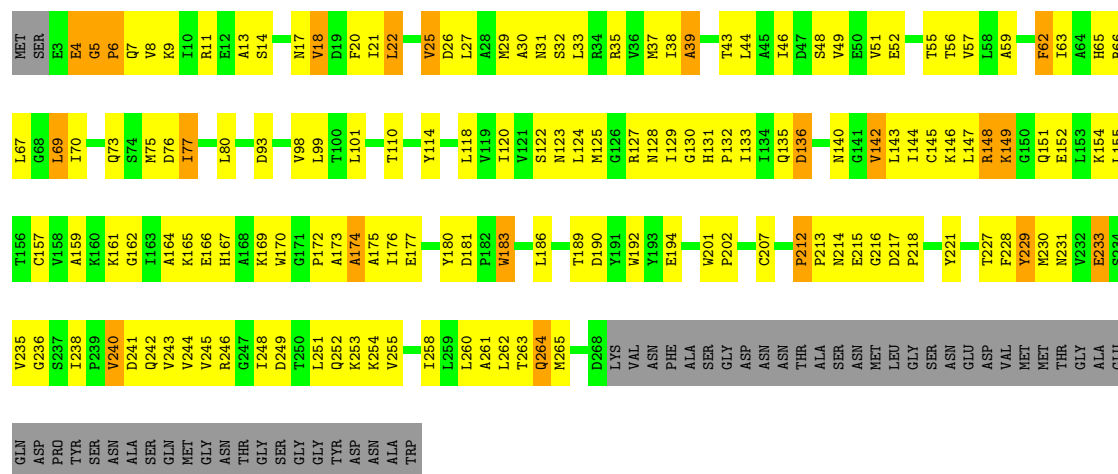






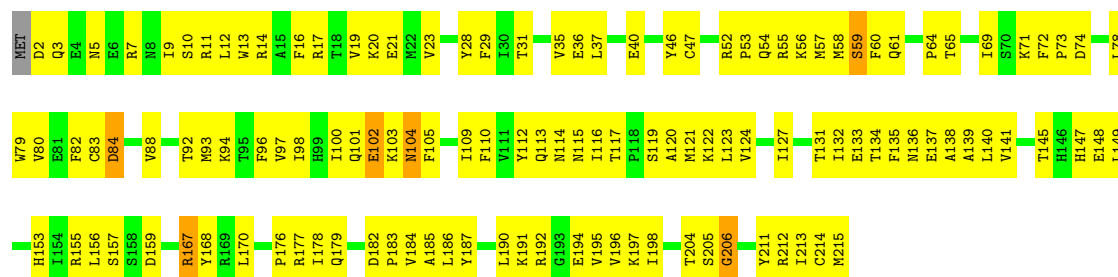
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

Chain C:



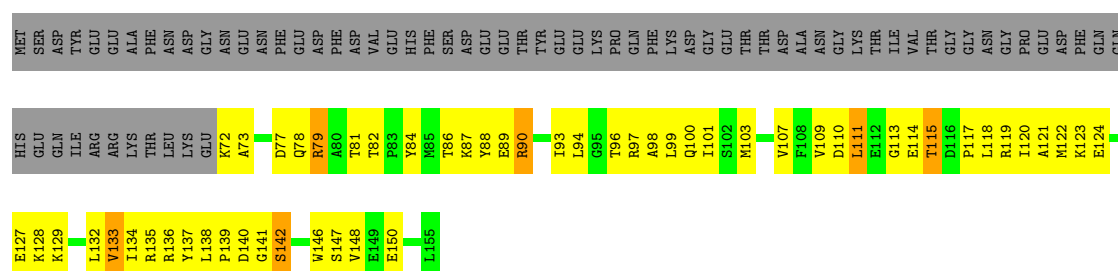
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E:



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F:



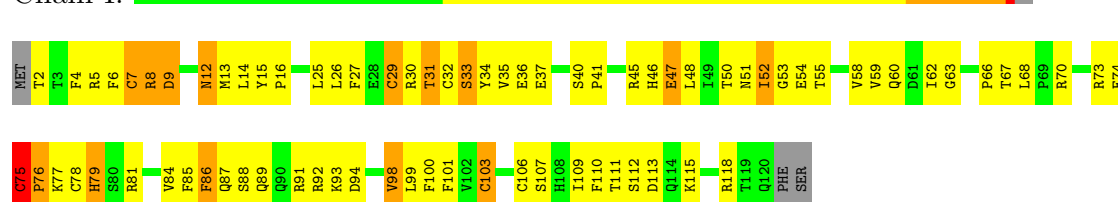
- Molecule 8: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H:



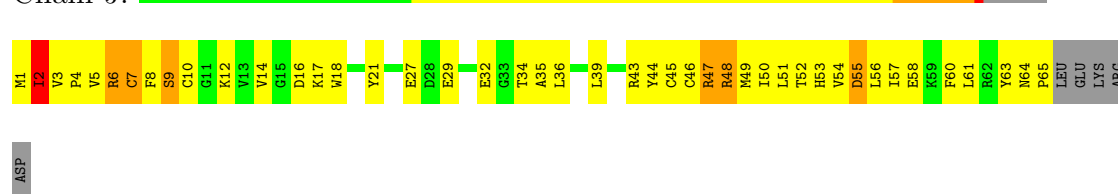
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I:



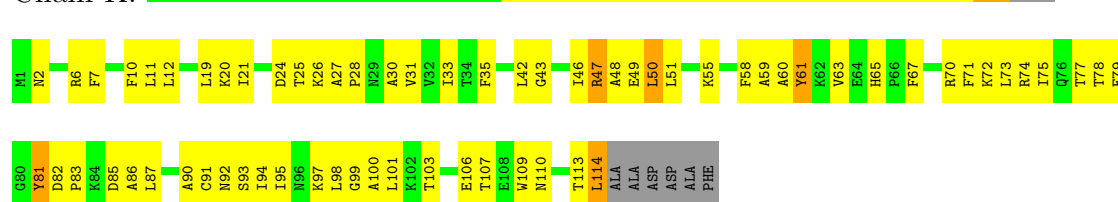
- Molecule 10: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J:



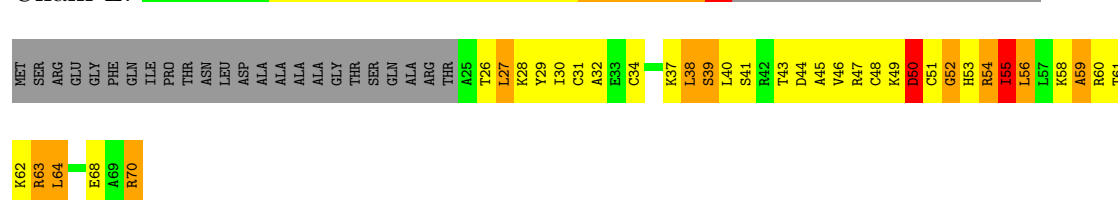
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

Chain K:



- Molecule 12: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.30Å 220.70Å 191.30Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.30)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.250 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	D	1.10	1/298 (0.3%)	1.03	0/456
2	R	1.70	4/219 (1.8%)	1.77	9/338 (2.7%)
3	A	0.41	0/11048	0.71	6/14936 (0.0%)
4	B	0.46	0/8891	0.71	2/11990 (0.0%)
5	C	0.48	0/2133	0.76	2/2891 (0.1%)
6	E	0.36	0/1788	0.65	0/2406
7	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.47	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.45	0/937	0.68	0/1265
12	L	0.48	0/366	0.78	0/485
All	All	0.47	5/28987 (0.0%)	0.73	20/39228 (0.1%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	9	A	P-OP2	7.91	1.62	1.49
2	R	1	G	OP3-P	-7.91	1.51	1.61
1	D	1	DA	OP3-P	-6.84	1.52	1.61
2	R	9	A	P-OP1	6.39	1.59	1.49
2	R	9	A	C2'-O2'	5.17	1.48	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	9	A	N9-C1'-C2'	-14.41	95.27	114.00
2	R	3	C	O5'-P-OP2	12.38	125.55	110.70
3	A	1392	SER	N-CA-C	6.34	128.11	111.00
2	R	3	C	C5'-C4'-O4'	6.26	116.61	109.10
2	R	9	A	C1'-O4'-C4'	-6.17	104.97	109.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	DA	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	267	0	148	30	0
2	R	196	0	100	26	0
3	A	10857	0	10959	1050	0
4	B	8721	0	8746	897	0
5	C	2095	0	2052	167	0
6	E	1752	0	1776	130	0
7	F	679	0	701	62	0
8	H	1068	0	1040	136	0
9	I	971	0	933	101	0
10	J	532	0	544	77	0
11	K	919	0	929	87	0
12	L	364	0	388	55	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	1	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	R	1	0	0	0	0
All	All	28430	0	28316	2555	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

The worst 5 of 2555 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.13
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.13
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1365/1733 (79%)	1021 (75%)	253 (18%)	91 (7%)	2	18
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	2	20
5	C	264/318 (83%)	208 (79%)	39 (15%)	17 (6%)	2	20
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	4	34
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	5	39
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	1	5
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	14
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	2	20
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	25	76
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	0
All	All	3465/4173 (83%)	2654 (77%)	583 (17%)	228 (7%)	2	19

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET

### 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	
3	A	1206/1520 (79%)	1129 (94%)	77 (6%)	25	69
4	B	952/1061 (90%)	886 (93%)	66 (7%)	22	67
5	C	234/274 (85%)	222 (95%)	12 (5%)	33	77
6	E	196/197 (100%)	189 (96%)	7 (4%)	47	85
7	F	74/137 (54%)	68 (92%)	6 (8%)	17	58
8	H	117/128 (91%)	112 (96%)	5 (4%)	40	82
9	I	113/116 (97%)	104 (92%)	9 (8%)	17	58
10	J	60/65 (92%)	56 (93%)	4 (7%)	23	67
11	K	99/102 (97%)	90 (91%)	9 (9%)	14	49
12	L	40/57 (70%)	35 (88%)	5 (12%)	7	31
All	All	3091/3657 (84%)	2891 (94%)	200 (6%)	24	69

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	268	THR
4	B	644	GLU
10	J	47	ARG
4	B	313	MET
4	B	466	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	325	GLN
4	B	538	ASN
9	I	12	ASN
4	B	363	HIS
4	B	515	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	9	A

There are no RNA pucker outliers to report.

## 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.