



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:03 am GMT

PDB ID : 7Z42  
Title : Influenza B polymerase with Pol II pSer5 CTD peptide mimic bound in site 2B  
Authors : Cusack, S.; Drncova, P.  
Deposited on : 2022-03-03  
Resolution : 2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

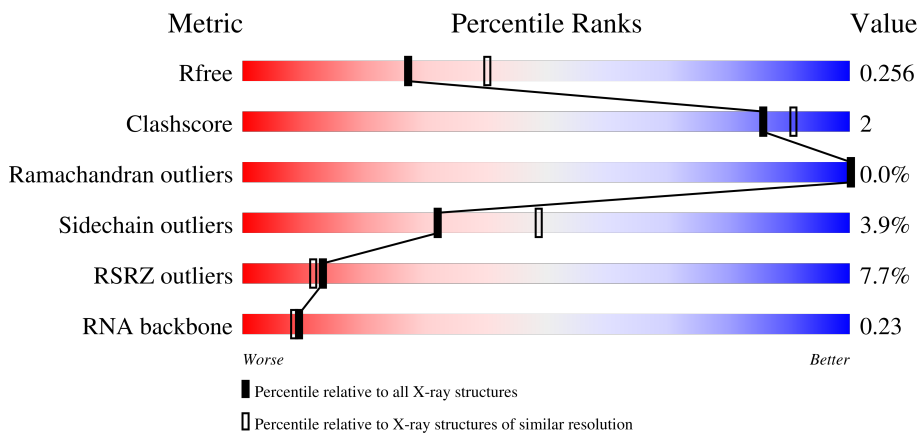
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)
RNA backbone	3102	1080 (2.80-2.04)

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 of 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  $\leq 5\%$ . 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	751	
1	D	751	
2	B	772	
2	E	772	

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Mol	Chain	Length	Quality of chain
3	C	798	<p>15% 82% 8% • 10%</p>
3	F	798	<p>18% 82% 8% • 9%</p>
4	G	28	<p>11% 75% 25%</p>
4	I	28	<p>4% 64% 36%</p>
4	X	28	<p>11% 14% 86%</p>
4	Y	28	<p>7% 7% • 89%</p>
5	H	13	<p>46% 46% 8%</p>
5	V	13	<p>46% 54%</p>

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 35949 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	721	5787	3675	970	1101	41	0	1	0
1	D	715	5750	3652	962	1095	41	0	1	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	GLY	-	expression tag	UNP Q5V8Z9
D	-12	SER	-	expression tag	UNP Q5V8Z9
D	-11	HIS	-	expression tag	UNP Q5V8Z9
D	-10	HIS	-	expression tag	UNP Q5V8Z9
D	-9	HIS	-	expression tag	UNP Q5V8Z9
D	-8	HIS	-	expression tag	UNP Q5V8Z9
D	-7	HIS	-	expression tag	UNP Q5V8Z9
D	-6	HIS	-	expression tag	UNP Q5V8Z9
D	-5	HIS	-	expression tag	UNP Q5V8Z9
D	-4	HIS	-	expression tag	UNP Q5V8Z9
D	-3	GLY	-	expression tag	UNP Q5V8Z9
D	-2	SER	-	expression tag	UNP Q5V8Z9
D	-1	GLY	-	expression tag	UNP Q5V8Z9
D	0	SER	-	expression tag	UNP Q5V8Z9
D	727	GLY	-	expression tag	UNP Q5V8Z9
D	728	SER	-	expression tag	UNP Q5V8Z9
D	729	GLY	-	expression tag	UNP Q5V8Z9
D	730	SER	-	expression tag	UNP Q5V8Z9
D	731	GLY	-	expression tag	UNP Q5V8Z9
D	732	GLU	-	expression tag	UNP Q5V8Z9
D	733	ASN	-	expression tag	UNP Q5V8Z9
D	734	LEU	-	expression tag	UNP Q5V8Z9
D	735	TYR	-	expression tag	UNP Q5V8Z9
D	736	PHE	-	expression tag	UNP Q5V8Z9
D	737	GLN	-	expression tag	UNP Q5V8Z9

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	754	5911	3731	1024	1104	52	0	0	0
2	E	743	5818	3671	1004	1091	52	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6
E	-8	GLY	-	expression tag	UNP Q5V8Y6
E	-7	SER	-	expression tag	UNP Q5V8Y6
E	-6	GLY	-	expression tag	UNP Q5V8Y6
E	-5	SER	-	expression tag	UNP Q5V8Y6
E	-4	GLY	-	expression tag	UNP Q5V8Y6
E	-3	SER	-	expression tag	UNP Q5V8Y6
E	-2	GLY	-	expression tag	UNP Q5V8Y6
E	-1	SER	-	expression tag	UNP Q5V8Y6
E	0	GLY	-	expression tag	UNP Q5V8Y6
E	753	GLY	-	expression tag	UNP Q5V8Y6
E	754	SER	-	expression tag	UNP Q5V8Y6
E	755	GLY	-	expression tag	UNP Q5V8Y6
E	756	SER	-	expression tag	UNP Q5V8Y6
E	757	GLY	-	expression tag	UNP Q5V8Y6
E	758	GLU	-	expression tag	UNP Q5V8Y6
E	759	ASN	-	expression tag	UNP Q5V8Y6
E	760	LEU	-	expression tag	UNP Q5V8Y6
E	761	TYR	-	expression tag	UNP Q5V8Y6
E	762	PHE	-	expression tag	UNP Q5V8Y6
E	763	GLN	-	expression tag	UNP Q5V8Y6

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	718	5746	3654	1001	1051	40	0	0	0
3	F	728	5838	3712	1023	1063	40	0	1	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	GLY	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3
F	-8	GLY	-	expression tag	UNP Q5V8X3
F	-7	SER	-	expression tag	UNP Q5V8X3
F	-6	GLY	-	expression tag	UNP Q5V8X3
F	-5	SER	-	expression tag	UNP Q5V8X3
F	-4	GLY	-	expression tag	UNP Q5V8X3
F	-3	SER	-	expression tag	UNP Q5V8X3
F	-2	GLY	-	expression tag	UNP Q5V8X3
F	-1	SER	-	expression tag	UNP Q5V8X3
F	0	GLY	-	expression tag	UNP Q5V8X3
F	771	GLY	-	expression tag	UNP Q5V8X3
F	772	TRP	-	expression tag	UNP Q5V8X3
F	773	SER	-	expression tag	UNP Q5V8X3
F	774	HIS	-	expression tag	UNP Q5V8X3
F	775	PRO	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	776	GLN	-	expression tag	UNP Q5V8X3
F	777	PHE	-	expression tag	UNP Q5V8X3
F	778	GLU	-	expression tag	UNP Q5V8X3
F	779	LYS	-	expression tag	UNP Q5V8X3
F	780	GLY	-	expression tag	UNP Q5V8X3
F	781	SER	-	expression tag	UNP Q5V8X3
F	782	GLY	-	expression tag	UNP Q5V8X3
F	783	SER	-	expression tag	UNP Q5V8X3
F	784	GLU	-	expression tag	UNP Q5V8X3
F	785	ASN	-	expression tag	UNP Q5V8X3
F	786	LEU	-	expression tag	UNP Q5V8X3
F	787	TYR	-	expression tag	UNP Q5V8X3
F	788	PHE	-	expression tag	UNP Q5V8X3
F	789	GLN	-	expression tag	UNP Q5V8X3

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	3	Total	C	N	O	P	0	0	0
			24	12	3	8	1			
4	G	21	Total	C	N	O	P	0	0	0
			165	96	21	45	3			
4	X	4	Total	C	N	O	P	0	0	0
			30	15	4	10	1			
4	I	18	Total	C	N	O	P	0	0	0
			142	85	18	37	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	13	Total	C	N	O	P	0	0	0
			266	117	52	84	13			
5	V	13	Total	C	N	O	P	0	0	0
			266	117	52	84	13			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		

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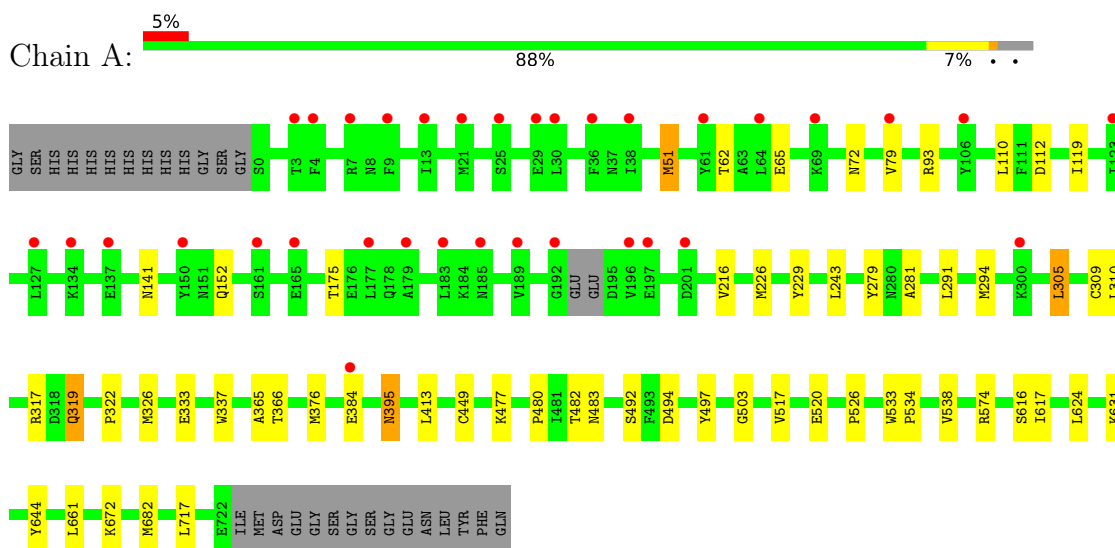
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	B	30	Total O 30 30	0	0
6	C	20	Total O 20 20	0	0
6	D	39	Total O 39 39	0	0
6	E	43	Total O 43 43	0	0
6	F	16	Total O 16 16	0	0
6	G	1	Total O 1 1	0	0
6	H	6	Total O 6 6	0	0
6	I	1	Total O 1 1	0	0
6	V	7	Total O 7 7	0	0

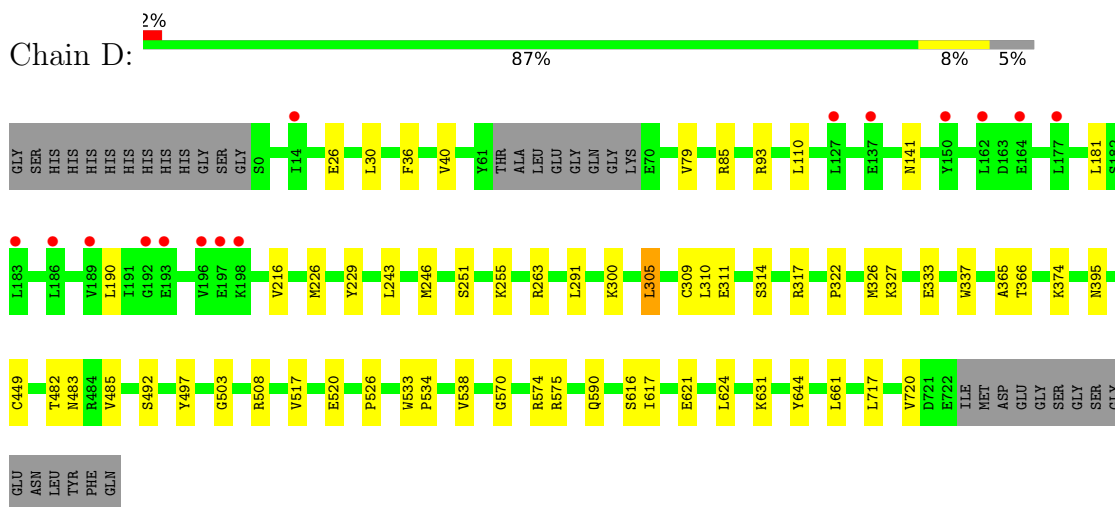
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

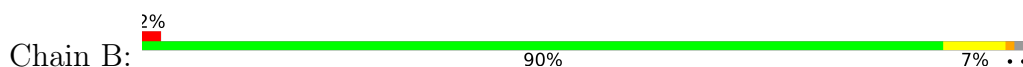
- Molecule 1: Polymerase acidic protein

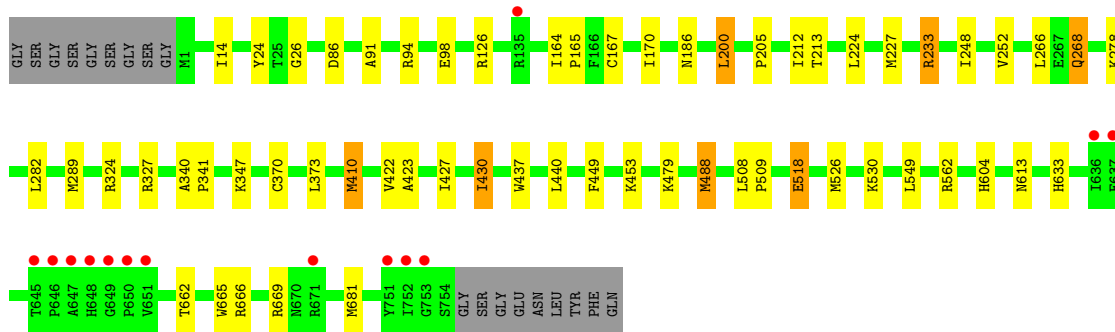


- Molecule 1: Polymerase acidic protein

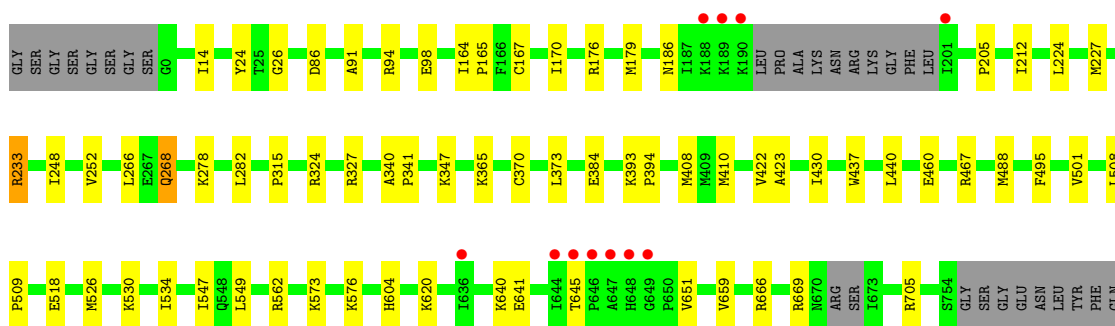
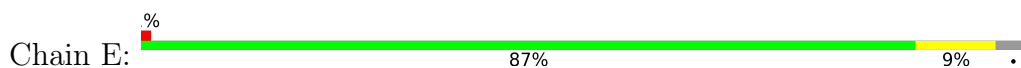


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

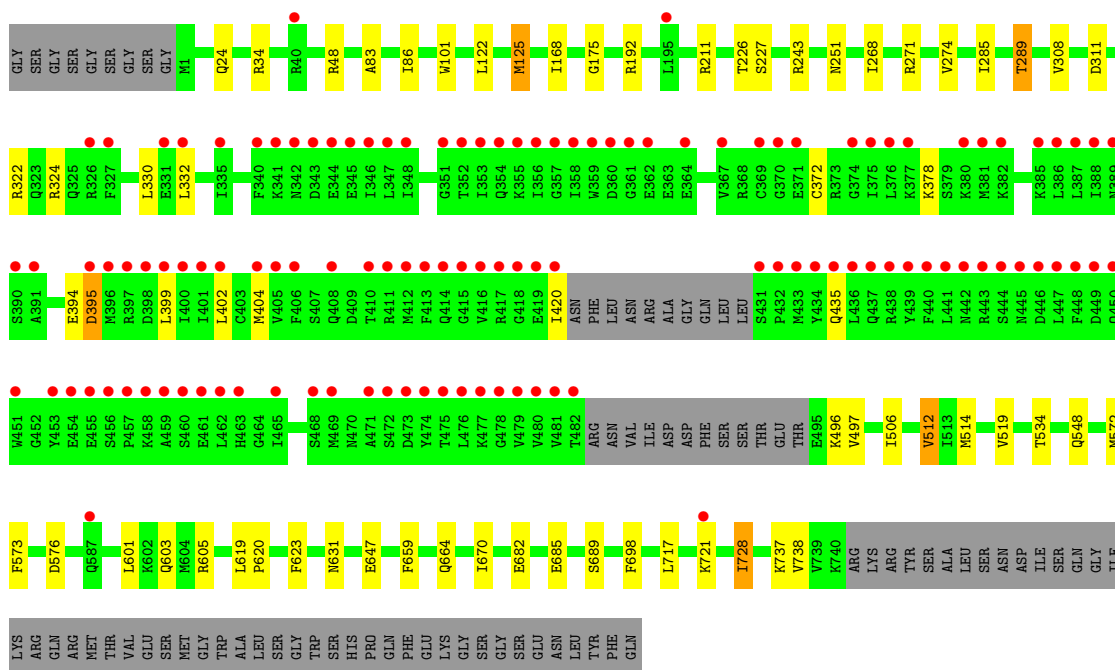
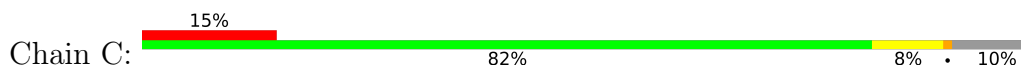




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

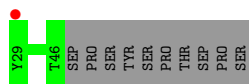


• Molecule 3: Polymerase basic protein 2

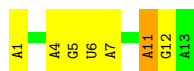


• Molecule 3: Polymerase basic protein 2

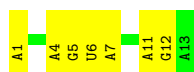




- Molecule 5: RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*AP\*CP\*AP\*AP\*GP\*A)-3')



- Molecule 5: RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*AP\*CP\*AP\*AP\*GP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.93Å 202.27Å 135.73Å 90.00° 110.54° 90.00°	Depositor
Resolution (Å)	127.11 – 2.42 127.11 – 2.42	Depositor EDS
% Data completeness (in resolution range)	61.4 (127.11-2.42) 61.4 (127.11-2.42)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.223 , 0.257 0.224 , 0.256	Depositor DCC
$R_{free}$ test set	7573 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtrriage
Anisotropy	0.059	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.001 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	35949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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 i

### 5.1 Standard geometry i

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

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	0.67	0/5903	0.71	0/7959
1	D	0.67	0/5866	0.70	0/7910
2	B	0.67	0/6028	0.71	0/8127
2	E	0.67	0/5931	0.71	0/7995
3	C	0.67	0/5844	0.72	0/7852
3	F	0.67	0/5939	0.72	0/7982
4	G	0.60	0/140	0.63	0/189
4	I	0.62	0/127	0.63	0/173
4	X	0.71	0/20	0.59	0/27
4	Y	0.57	0/14	0.80	0/18
5	H	0.93	1/298 (0.3%)	1.26	3/462 (0.6%)
5	V	0.93	1/298 (0.3%)	1.25	2/462 (0.4%)
All	All	0.67	2/36408 (0.0%)	0.73	5/49156 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	A	OP3-P	-7.51	1.52	1.61
5	H	1	A	OP3-P	-7.43	1.52	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	5	G	P-O3'-C3'	-6.80	111.54	119.70
5	H	12	G	P-O3'-C3'	-6.47	111.93	119.70
5	H	5	G	P-O3'-C3'	-6.04	112.45	119.70
5	H	6	U	P-O3'-C3'	-5.63	112.95	119.70
5	V	6	U	P-O3'-C3'	-5.56	113.03	119.70

There are no chirality outliers.

There are no planarity outliers.

## 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	5787	0	5761	33	0
1	D	5750	0	5717	28	0
2	B	5911	0	5932	30	0
2	E	5818	0	5824	34	0
3	C	5746	0	5909	25	0
3	F	5838	0	6007	33	0
4	G	165	0	130	0	0
4	I	142	0	115	0	0
4	X	30	0	21	0	0
4	Y	24	0	17	1	0
5	H	266	0	130	1	0
5	V	266	0	130	1	0
6	A	43	0	0	0	0
6	B	30	0	0	0	0
6	C	20	0	0	0	0
6	D	39	0	0	0	0
6	E	43	0	0	1	0
6	F	16	0	0	0	0
6	G	1	0	0	0	0
6	H	6	0	0	0	0
6	I	1	0	0	0	0
6	V	7	0	0	0	0
All	All	35949	0	35693	160	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 2.

All (160) 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:A:51:MET:O	1:A:62:THR:HA	1.92	0.70
2:B:282:LEU:HD22	2:B:440:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:717:LEU:HD21	3:F:728:ILE:HD11	1.77	0.66
2:E:282:LEU:HD22	2:E:440:LEU:HD13	1.78	0.66
3:F:273:ILE:HD11	3:F:516:ALA:CB	2.26	0.66
1:A:616:SER:HB3	1:A:624:LEU:HD21	1.78	0.65
1:D:590:GLN:HE21	3:F:241:ASN:HD21	1.45	0.65
1:D:483:ASN:HB2	1:D:497:TYR:HE2	1.61	0.65
1:A:483:ASN:HB2	1:A:497:TYR:HE2	1.62	0.64
3:F:273:ILE:HD11	3:F:516:ALA:HB1	1.83	0.61
3:F:609:VAL:HA	3:F:688:ARG:HD3	1.84	0.59
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.85	0.58
1:A:319:GLN:HA	1:A:319:GLN:HE21	1.67	0.58
2:E:340:ALA:HB3	2:E:341:PRO:HD3	1.86	0.58
2:E:526:MET:HE1	2:E:547:ILE:HG23	1.87	0.57
2:E:224:LEU:HD11	2:E:347:LYS:HD2	1.88	0.56
3:C:506:ILE:HD13	3:C:512:VAL:HB	1.89	0.55
3:F:603:GLN:NE2	3:F:698:PHE:O	2.40	0.55
3:F:372:CYS:HB3	3:F:399:LEU:HD13	1.89	0.54
3:C:603:GLN:NE2	3:C:698:PHE:O	2.40	0.54
3:C:717:LEU:HD11	3:C:728:ILE:HD11	1.88	0.54
2:B:24:TYR:CE1	2:B:233:ARG:HG2	2.44	0.53
2:E:24:TYR:CE1	2:E:233:ARG:HG2	2.44	0.53
1:D:717:LEU:HG	3:F:664:GLN:HB2	1.91	0.52
2:B:266:LEU:HD13	2:B:422:VAL:HG11	1.90	0.52
2:E:266:LEU:HD13	2:E:422:VAL:HG11	1.90	0.52
2:B:224:LEU:HD13	2:B:410:MET:HG3	1.92	0.52
2:E:26:GLY:O	2:E:233:ARG:NH2	2.43	0.51
2:E:530:LYS:HE2	2:E:604:HIS:HB3	1.92	0.51
2:B:268:GLN:CG	2:B:422:VAL:HG13	2.41	0.51
3:C:122:LEU:O	3:C:125:MET:HG3	2.11	0.51
3:F:607:GLN:HG2	3:F:699:LEU:HD11	1.92	0.51
2:B:26:GLY:O	2:B:233:ARG:NH2	2.43	0.51
2:B:24:TYR:CZ	2:B:233:ARG:HG2	2.45	0.50
3:C:717:LEU:HD21	3:C:728:ILE:HD11	1.93	0.50
1:D:229:TYR:OH	2:E:86:ASP:OD1	2.27	0.50
2:E:24:TYR:CZ	2:E:233:ARG:HG2	2.45	0.50
3:F:122:LEU:O	3:F:125:MET:HG3	2.12	0.50
2:E:573:LYS:HD3	3:F:77:ILE:HD11	1.92	0.50
1:A:366:THR:HG23	1:A:503:GLY:HA3	1.94	0.50
3:F:401:ILE:O	3:F:405:VAL:HG23	2.12	0.50
2:B:91:ALA:HB1	2:B:423:ALA:HB1	1.94	0.49
1:D:366:THR:HG23	1:D:503:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:654:LYS:HG2	3:F:731:TYR:HB3	1.95	0.49
1:A:717:LEU:HG	3:C:664:GLN:HB2	1.94	0.49
1:A:480:PRO:HB2	1:A:482:THR:HG23	1.93	0.49
2:B:167:CYS:HA	2:B:170:ILE:HD12	1.94	0.49
1:D:36:PHE:CE2	1:D:190:LEU:HD21	2.47	0.49
1:D:374:LYS:HA	2:E:365:LYS:O	2.13	0.49
2:E:268:GLN:CG	2:E:422:VAL:HG13	2.43	0.49
2:E:167:CYS:HA	2:E:170:ILE:HD12	1.94	0.49
2:E:91:ALA:HB1	2:E:423:ALA:HB1	1.96	0.48
3:C:308:VAL:HG13	3:C:514:MET:HG2	1.95	0.48
1:A:661:LEU:HD13	1:A:682:MET:HE1	1.96	0.48
1:D:181:LEU:HD13	1:D:190:LEU:HD22	1.96	0.48
1:D:533:TRP:N	1:D:534:PRO:CD	2.77	0.47
1:A:243:LEU:CD1	2:B:430:ILE:HG12	2.45	0.47
1:A:322:PRO:HG3	1:A:337:TRP:CE2	2.49	0.47
1:A:533:TRP:N	1:A:534:PRO:CD	2.77	0.47
1:A:413:LEU:HD12	4:Y:26:SEP:HB3	1.96	0.47
2:E:370:CYS:HA	2:E:373:LEU:HD13	1.96	0.47
1:A:79:VAL:HA	1:A:110:LEU:HD23	1.97	0.47
1:D:574:ARG:HB3	2:E:549:LEU:HD22	1.96	0.47
3:F:346:ILE:HD11	3:F:358:ILE:HD11	1.96	0.46
2:B:186:ASN:HA	2:B:205:PRO:HA	1.97	0.46
2:B:370:CYS:HA	2:B:373:LEU:HD13	1.96	0.46
1:A:229:TYR:OH	2:B:86:ASP:OD1	2.31	0.46
1:D:322:PRO:HG3	1:D:337:TRP:CE2	2.49	0.46
2:E:186:ASN:HA	2:E:205:PRO:HA	1.97	0.46
1:D:575:ARG:NH1	6:E:802:HOH:O	2.49	0.46
1:A:279:TYR:CE1	1:A:281:ALA:HB3	2.51	0.46
3:F:551:TYR:HB3	3:F:670:ILE:HD13	1.98	0.46
1:A:672:LYS:HG3	2:B:488:MET:HE3	1.98	0.45
3:C:311:ASP:OD1	3:C:322:ARG:O	2.35	0.45
1:D:644:TYR:HA	2:E:26:GLY:HA2	1.98	0.45
1:A:661:LEU:HD13	1:A:682:MET:CE	2.45	0.45
1:A:574:ARG:HB3	2:B:549:LEU:HD22	1.99	0.45
3:C:372:CYS:HB3	3:C:399:LEU:HD22	1.99	0.45
1:A:305:LEU:C	1:A:305:LEU:HD12	2.37	0.45
3:F:311:ASP:OD1	3:F:322:ARG:O	2.33	0.45
1:D:79:VAL:HA	1:D:110:LEU:HD23	2.00	0.45
2:B:200:LEU:HD11	5:V:12:G:C2	2.52	0.44
3:C:682:GLU:O	3:C:685:GLU:HB3	2.17	0.44
1:A:682:MET:HG3	2:B:479:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:GLU:HG2	2:B:665:TRP:CZ2	2.52	0.44
3:C:573:PHE:O	3:C:623:PHE:HA	2.17	0.44
3:F:573:PHE:O	3:F:623:PHE:HA	2.16	0.44
1:D:305:LEU:C	1:D:305:LEU:HD12	2.38	0.44
1:D:720:VAL:HG21	3:F:663:PRO:HG2	2.00	0.44
2:E:534:ILE:O	3:F:142:ARG:NH2	2.47	0.44
1:A:672:LYS:HG3	2:B:488:MET:CE	2.47	0.44
2:E:659:VAL:HG11	3:F:113:PHE:CZ	2.53	0.44
1:A:291:LEU:O	1:A:309[A]:CYS:SG	2.76	0.43
1:D:291:LEU:O	1:D:309[A]:CYS:SG	2.76	0.43
3:C:619:LEU:HB3	3:C:620:PRO:HD3	2.00	0.43
2:B:278:LYS:O	2:B:282:LEU:HG	2.19	0.43
3:C:394:GLU:HG3	3:C:395:ASP:OD1	2.19	0.43
2:E:659:VAL:HG11	3:F:113:PHE:HZ	1.84	0.43
1:D:93:ARG:HD2	3:F:175:GLY:O	2.19	0.43
1:A:644:TYR:HA	2:B:26:GLY:HA2	1.99	0.43
2:E:508:LEU:HB3	2:E:509:PRO:HD3	2.00	0.43
1:A:395:ASN:OD1	1:A:395:ASN:N	2.51	0.42
3:C:308:VAL:HG12	3:C:519:VAL:HG12	2.01	0.42
2:E:640:LYS:HG3	2:E:641:GLU:N	2.34	0.42
3:F:698:PHE:HB3	3:F:738:VAL:CG1	2.48	0.42
3:F:190:GLU:OE2	3:F:194:LYS:NZ	2.52	0.42
1:A:152:GLN:NE2	1:A:175:THR:OG1	2.50	0.42
1:A:310:LEU:HB3	1:A:317:ARG:HG3	2.01	0.42
2:B:530:LYS:HE2	2:B:604:HIS:HB3	2.01	0.42
3:C:285:ILE:O	3:C:289:THR:HG23	2.19	0.42
3:C:83:ALA:HA	3:C:86:ILE:HD12	2.02	0.42
3:F:619:LEU:HB3	3:F:620:PRO:HD3	2.01	0.42
3:F:658:LEU:O	3:F:670:ILE:HA	2.20	0.42
1:A:93:ARG:HD2	3:C:175:GLY:O	2.19	0.42
1:A:216:VAL:HG12	1:A:226:MET:HE2	2.01	0.42
2:B:370:CYS:O	2:B:373:LEU:HB2	2.19	0.42
1:A:661:LEU:HD12	1:A:661:LEU:HA	1.92	0.42
1:D:508:ARG:NH2	5:H:11:A:N3	2.68	0.42
1:D:526:PRO:HG3	1:D:538:VAL:HG11	2.01	0.42
2:E:645:THR:HG22	2:E:651:VAL:HG22	2.01	0.42
3:F:705:ASP:HB2	3:F:737:LYS:HE3	2.01	0.42
1:D:310:LEU:HB3	1:D:317:ARG:HG3	2.01	0.42
3:F:654:LYS:CG	3:F:731:TYR:HB3	2.50	0.42
2:B:289:MET:HG2	2:B:449:PHE:HB3	2.01	0.41
3:C:168:ILE:HA	3:C:192:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:698:PHE:HB3	3:C:738:VAL:CG1	2.49	0.41
3:F:268:ILE:HD11	3:F:289:THR:HG21	2.02	0.41
3:F:285:ILE:O	3:F:289:THR:HG23	2.20	0.41
2:E:176:ARG:HG3	2:E:179:MET:HE2	2.02	0.41
3:C:268:ILE:HD11	3:C:289:THR:HG21	2.02	0.41
2:E:248:ILE:HG12	2:E:252:VAL:HG23	2.03	0.41
2:E:393:LYS:HB2	2:E:394:PRO:HD3	2.03	0.41
1:A:305:LEU:HD13	1:A:494:ASP:HB3	2.03	0.41
3:C:420:ILE:HD11	3:C:435:GLN:HB3	2.03	0.41
3:C:659:PHE:CD2	3:C:670:ILE:CD1	3.03	0.41
1:D:246:MET:HE2	2:E:467:ARG:HB3	2.02	0.41
2:B:508:LEU:HB3	2:B:509:PRO:HD3	2.02	0.41
2:B:662:THR:HG21	3:C:101:TRP:CD1	2.55	0.41
3:C:330:LEU:HB2	3:C:402:LEU:HD13	2.03	0.41
1:D:616:SER:HB3	1:D:624:LEU:HD21	2.02	0.41
2:E:164:ILE:N	2:E:165:PRO:HD2	2.36	0.41
2:E:315:PRO:HG3	2:E:408:MET:CE	2.51	0.41
2:E:370:CYS:O	2:E:373:LEU:HB2	2.20	0.41
1:A:112:ASP:HB2	1:A:119:ILE:HD11	2.02	0.41
1:A:526:PRO:HG3	1:A:538:VAL:HG11	2.02	0.41
2:B:164:ILE:N	2:B:165:PRO:HD2	2.36	0.41
2:B:248:ILE:HG12	2:B:252:VAL:HG23	2.03	0.41
3:F:80:LYS:HA	3:F:93:CYS:HA	2.03	0.41
2:B:224:LEU:HD11	2:B:347:LYS:HD2	2.01	0.41
1:D:216:VAL:HG12	1:D:226:MET:HE2	2.03	0.41
3:F:682:GLU:O	3:F:685:GLU:HB3	2.21	0.41
1:A:365:ALA:HB1	1:A:517:VAL:HG21	2.03	0.40
1:D:365:ALA:HB1	1:D:517:VAL:HG21	2.04	0.40
3:C:211:ARG:HD2	3:C:211:ARG:HA	1.91	0.40
1:D:570:GLY:HA2	1:D:644:TYR:CZ	2.57	0.40
1:D:616:SER:CB	1:D:624:LEU:HD21	2.52	0.40
1:D:661:LEU:HD12	1:D:661:LEU:HA	1.90	0.40
3:F:34:ARG:O	3:F:34:ARG:HD3	2.22	0.40
2:E:278:LYS:O	2:E:282:LEU:HG	2.22	0.40
2:E:495:PHE:O	2:E:501:VAL:HG22	2.22	0.40

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	718/751 (96%)	691 (96%)	26 (4%)	1 (0%)	51	67
1	D	712/751 (95%)	688 (97%)	24 (3%)	0	100	100
2	B	752/772 (97%)	726 (96%)	26 (4%)	0	100	100
2	E	737/772 (96%)	714 (97%)	23 (3%)	0	100	100
3	C	712/798 (89%)	678 (95%)	34 (5%)	0	100	100
3	F	725/798 (91%)	693 (96%)	31 (4%)	1 (0%)	51	67
4	G	16/28 (57%)	16 (100%)	0	0	100	100
4	I	14/28 (50%)	13 (93%)	1 (7%)	0	100	100
4	X	2/28 (7%)	2 (100%)	0	0	100	100
4	Y	1/28 (4%)	1 (100%)	0	0	100	100
All	All	4389/4754 (92%)	4222 (96%)	165 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
3	F	89	LYS

### 5.3.2 Protein sidechains [i](#)

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	641/664 (96%)	624 (97%)	17 (3%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	638/664 (96%)	613 (96%)	25 (4%)	32	49
2	B	646/657 (98%)	620 (96%)	26 (4%)	31	48
2	E	636/657 (97%)	614 (96%)	22 (4%)	36	53
3	C	628/694 (90%)	597 (95%)	31 (5%)	25	39
3	F	637/694 (92%)	609 (96%)	28 (4%)	28	43
4	G	18/24 (75%)	18 (100%)	0	100	100
4	I	16/24 (67%)	16 (100%)	0	100	100
4	X	3/24 (12%)	3 (100%)	0	100	100
4	Y	2/24 (8%)	2 (100%)	0	100	100
All	All	3865/4126 (94%)	3716 (96%)	149 (4%)	32	49

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	MET
1	A	72	ASN
1	A	141	ASN
1	A	294	MET
1	A	305	LEU
1	A	319	GLN
1	A	326	MET
1	A	333	GLU
1	A	376	MET
1	A	384	GLU
1	A	395	ASN
1	A	449	CYS
1	A	477	LYS
1	A	492	SER
1	A	520	GLU
1	A	617	ILE
1	A	631	LYS
2	B	14	ILE
2	B	94	ARG
2	B	98	GLU
2	B	126	ARG
2	B	200	LEU
2	B	212	ILE
2	B	213	THR
2	B	227	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	233	ARG
2	B	268	GLN
2	B	324	ARG
2	B	327	ARG
2	B	410	MET
2	B	427	ILE
2	B	430	ILE
2	B	437	TRP
2	B	453	LYS
2	B	488	MET
2	B	518	GLU
2	B	526	MET
2	B	562	ARG
2	B	613	ASN
2	B	633	HIS
2	B	666	ARG
2	B	669	ARG
2	B	681	MET
3	C	24	GLN
3	C	34	ARG
3	C	48	ARG
3	C	125	MET
3	C	226	THR
3	C	227	SER
3	C	243	ARG
3	C	251	ASN
3	C	271	ARG
3	C	274	VAL
3	C	289	THR
3	C	324	ARG
3	C	332	LEU
3	C	378	LYS
3	C	395	ASP
3	C	404	MET
3	C	496	LYS
3	C	497	VAL
3	C	512	VAL
3	C	534	THR
3	C	548	GLN
3	C	572	MET
3	C	576	ASP
3	C	601	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	605	ARG
3	C	631	ASN
3	C	647	GLU
3	C	689	SER
3	C	721	LYS
3	C	728	ILE
3	C	737	LYS
1	D	26	GLU
1	D	30	LEU
1	D	40	VAL
1	D	85	ARG
1	D	141	ASN
1	D	243	LEU
1	D	251	SER
1	D	255	LYS
1	D	263	ARG
1	D	300	LYS
1	D	305	LEU
1	D	311	GLU
1	D	314	SER
1	D	326	MET
1	D	327	LYS
1	D	333	GLU
1	D	395	ASN
1	D	449	CYS
1	D	482	THR
1	D	485	VAL
1	D	492	SER
1	D	520	GLU
1	D	617	ILE
1	D	621	GLU
1	D	631	LYS
2	E	14	ILE
2	E	94	ARG
2	E	98	GLU
2	E	212	ILE
2	E	227	MET
2	E	233	ARG
2	E	268	GLN
2	E	324	ARG
2	E	327	ARG
2	E	384	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	410	MET
2	E	430	ILE
2	E	437	TRP
2	E	460	GLU
2	E	488	MET
2	E	518	GLU
2	E	562	ARG
2	E	576	LYS
2	E	620	LYS
2	E	666	ARG
2	E	669	ARG
2	E	705	ARG
3	F	34	ARG
3	F	125	MET
3	F	226	THR
3	F	271	ARG
3	F	273	ILE
3	F	274	VAL
3	F	289	THR
3	F	332	LEU
3	F	340	PHE
3	F	368	ARG
3	F	372	CYS
3	F	378	LYS
3	F	422	PHE
3	F	504	SER
3	F	512	VAL
3	F	523	GLU
3	F	534	THR
3	F	552	GLN
3	F	572	MET
3	F	576	ASP
3	F	601	LEU
3	F	605	ARG
3	F	607	GLN
3	F	624	SER
3	F	647	GLU
3	F	689	SER
3	F	732	GLN
3	F	737	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
2	B	613	ASN
3	C	631	ASN
1	D	590	GLN
2	E	310	ASN
3	F	325	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	H	11/13 (84%)	3 (27%)	0
5	V	11/13 (84%)	3 (27%)	0
All	All	22/26 (84%)	6 (27%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	H	4	A
5	H	7	A
5	H	11	A
5	V	4	A
5	V	7	A
5	V	11	A

There are no RNA pucker outliers to report.

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

7 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	$\# Z  > 2$
4	SEP	G	47	4	8,9,10	0.54	0	8,12,14	0.64	0
4	SEP	G	33	4	8,9,10	0.56	0	8,12,14	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SEP	I	33	4	8,9,10	0.56	0	8,12,14	0.62	0
4	SEP	X	26	4	8,9,10	0.55	0	8,12,14	0.68	0
4	SEP	Y	26	4	8,9,10	0.57	0	8,12,14	0.64	0
4	SEP	I	40	4	8,9,10	0.51	0	8,12,14	0.64	0
4	SEP	G	40	4	8,9,10	0.72	0	8,12,14	0.63	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
4	SEP	G	47	4	-	2/5/8/10	-
4	SEP	G	33	4	-	2/5/8/10	-
4	SEP	I	33	4	-	2/5/8/10	-
4	SEP	X	26	4	-	1/5/8/10	-
4	SEP	Y	26	4	-	1/5/8/10	-
4	SEP	I	40	4	-	0/5/8/10	-
4	SEP	G	40	4	-	4/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	40	SEP	CB-OG-P-O1P
4	G	40	SEP	CB-OG-P-O2P
4	G	40	SEP	CB-OG-P-O3P
4	Y	26	SEP	N-CA-CB-OG
4	X	26	SEP	N-CA-CB-OG
4	G	40	SEP	CA-CB-OG-P
4	G	47	SEP	CA-CB-OG-P
4	G	33	SEP	N-CA-CB-OG
4	G	47	SEP	N-CA-CB-OG
4	I	33	SEP	N-CA-CB-OG
4	G	33	SEP	CA-CB-OG-P
4	I	33	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	26	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	721/751 (96%)	0.34	34 (4%) 31 29	21, 40, 126, 149	0
1	D	715/751 (95%)	0.22	15 (2%) 63 60	23, 39, 116, 139	0
2	B	754/772 (97%)	0.15	14 (1%) 66 64	23, 45, 76, 116	0
2	E	743/772 (96%)	0.16	11 (1%) 73 71	23, 42, 69, 110	0
3	C	718/798 (89%)	1.06	119 (16%) 1 1	25, 56, 185, 226	0
3	F	728/798 (91%)	1.24	140 (19%) 1 0	26, 54, 172, 193	0
4	G	18/28 (64%)	0.87	3 (16%) 1 1	46, 68, 131, 137	0
4	I	16/28 (57%)	0.69	1 (6%) 20 18	46, 63, 75, 89	0
4	X	3/28 (10%)	4.20	3 (100%) 0 0	94, 94, 96, 97	0
4	Y	2/28 (7%)	3.86	2 (100%) 0 0	98, 98, 98, 98	0
5	H	13/13 (100%)	-0.46	0 100 100	25, 29, 56, 69	0
5	V	13/13 (100%)	-0.39	0 100 100	25, 28, 40, 47	0
All	All	4444/4780 (92%)	0.53	342 (7%) 13 11	21, 46, 139, 226	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	425	ARG	25.0
3	F	423	LEU	22.2
3	C	460	SER	16.8
3	C	431	SER	16.0
3	C	419	GLU	14.7
3	F	422	PHE	14.5
3	F	426	ALA	14.5
3	C	441	LEU	14.4
3	F	429	LEU	14.2
3	F	460	SER	13.0
3	C	420	ILE	12.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	459	ALA	12.5
3	F	434	TYR	12.4
3	F	424	ASN	12.0
3	C	481	VAL	11.8
3	F	427	GLY	11.7
3	C	442	ASN	11.4
3	C	434	TYR	11.2
3	C	447	LEU	10.6
3	F	441	LEU	10.3
3	C	477	LYS	10.2
3	C	443	ARG	10.2
3	F	440	PHE	10.0
3	C	416	VAL	9.9
3	F	354	GLN	9.8
3	F	442	ASN	9.2
3	C	358	ILE	9.1
3	F	439	TYR	9.1
3	F	474	TYR	8.8
3	F	349	GLY	8.7
3	C	410	THR	8.7
3	C	340	PHE	8.4
3	C	413	PHE	8.3
3	C	386	LEU	8.2
3	C	468	SER	8.2
3	F	420	ILE	8.0
3	C	354	GLN	8.0
3	C	353	ILE	7.9
3	C	433	MET	7.8
3	F	384	GLU	7.8
3	F	397	ARG	7.8
3	C	471	ALA	7.7
3	C	356	ILE	7.5
3	F	418	GLY	7.5
3	F	326	ARG	7.5
3	F	385	LYS	7.5
3	C	414	GLN	7.4
3	C	440	PHE	7.3
3	C	455	GLU	7.3
3	F	468	SER	7.2
3	F	386	LEU	7.2
3	F	452	GLY	7.1
3	C	439	TYR	7.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	X	25	THR	7.1
3	C	347	LEU	7.0
3	C	458	LYS	7.0
3	C	451	TRP	7.0
3	F	431	SER	7.0
3	F	413	PHE	6.9
3	F	430	LEU	6.9
3	C	351	GLY	6.7
3	C	341	LYS	6.6
3	F	348	ILE	6.6
3	C	462	LEU	6.6
3	F	428	GLN	6.6
3	F	419	GLU	6.5
3	F	443	ARG	6.5
3	F	462	LEU	6.5
3	C	445	ASN	6.5
3	F	356	ILE	6.4
3	C	438	ARG	6.4
3	C	432	PRO	6.3
3	F	454	GLU	6.3
3	F	456	SER	6.3
3	C	444	SER	6.2
1	D	192	GLY	6.2
2	E	647	ALA	6.2
3	C	355	LYS	6.2
3	F	417	ARG	6.2
3	C	357	GLY	6.1
3	F	469	MET	6.1
2	E	648	HIS	6.0
3	F	438	ARG	5.9
3	C	436	LEU	5.9
3	C	473	ASP	5.8
3	F	473	ASP	5.8
3	F	448	PHE	5.8
3	F	471	ALA	5.8
3	F	347	LEU	5.8
3	C	406	PHE	5.8
3	F	455	GLU	5.7
3	F	351	GLY	5.7
4	Y	25	THR	5.7
3	F	403	CYS	5.7
3	C	459	ALA	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	387	LEU	5.6
3	C	457	PRO	5.6
3	C	387	LEU	5.6
3	F	421	ASN	5.5
3	C	398	ASP	5.5
3	F	383	LEU	5.5
3	F	451	TRP	5.4
3	F	463	HIS	5.4
3	C	346	ILE	5.3
3	F	447	LEU	5.3
1	A	201	ASP	5.2
3	F	343	ASP	5.2
3	F	482	THR	5.1
3	C	405	VAL	5.1
3	C	418	GLY	5.1
1	A	189	VAL	5.1
3	F	328	GLY	5.0
3	C	352	THR	5.0
3	C	448	PHE	5.0
3	F	480	VAL	5.0
3	F	88	THR	5.0
3	F	472	SER	4.9
3	F	476	LEU	4.8
3	F	402	LEU	4.8
3	F	410	THR	4.8
3	F	433	MET	4.8
3	F	437	GLN	4.8
3	F	373	ARG	4.8
3	F	405	VAL	4.7
3	F	416	VAL	4.7
3	C	476	LEU	4.7
3	F	375	ILE	4.7
3	F	406	PHE	4.7
3	F	87	GLY	4.6
3	F	346	ILE	4.6
3	F	478	GLY	4.6
3	F	342	ASN	4.6
3	C	348	ILE	4.5
3	C	345	GLU	4.5
3	C	435	GLN	4.5
3	F	396	MET	4.5
3	F	398	ASP	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	414	GLN	4.4
3	F	458	LYS	4.4
3	F	461	GLU	4.4
3	F	475	THR	4.4
3	C	390	SER	4.3
3	C	369	CYS	4.3
3	F	336	SER	4.3
3	F	444	SER	4.3
1	A	197	GLU	4.3
3	F	483	ARG	4.2
3	F	432	PRO	4.2
3	F	335	ILE	4.1
3	C	404	MET	4.1
3	C	391	ALA	4.1
3	F	399	LEU	4.1
3	C	474	TYR	4.1
3	F	86	ILE	4.1
3	F	376	LEU	4.1
3	F	353	ILE	4.0
2	B	751	TYR	4.0
3	F	340	PHE	4.0
1	A	185	ASN	4.0
3	C	396	MET	4.0
1	A	150	TYR	4.0
3	F	327	PHE	4.0
3	C	335	ILE	3.9
1	A	127	LEU	3.9
3	F	435	GLN	3.9
3	F	465	ILE	3.9
3	F	329	ARG	3.9
3	F	374	GLY	3.9
3	F	358	ILE	3.9
2	E	646	PRO	3.9
3	C	469	MET	3.8
3	F	391	ALA	3.8
3	F	400	ILE	3.8
3	C	342	ASN	3.8
3	C	362	GLU	3.7
3	F	404	MET	3.7
3	F	370	GLY	3.7
3	C	397	ARG	3.7
2	E	201	ILE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	587	GLN	3.7
3	C	417	ARG	3.6
1	D	177	LEU	3.6
3	F	332	LEU	3.6
4	I	29	TYR	3.6
3	C	446	ASP	3.6
3	C	482	THR	3.6
3	F	359	TRP	3.5
3	C	377	LYS	3.5
1	D	193	GLU	3.5
3	C	385	LYS	3.5
1	D	186	LEU	3.4
3	F	83	ALA	3.4
1	A	64	LEU	3.4
3	C	400	ILE	3.4
3	F	389	ASN	3.4
3	F	352	THR	3.4
1	A	134	LYS	3.4
3	C	478	GLY	3.3
3	C	359	TRP	3.3
1	D	196	VAL	3.3
3	F	470	ASN	3.3
3	C	370	GLY	3.3
3	C	480	VAL	3.3
3	F	477	LYS	3.3
3	C	360	ASP	3.3
3	C	399	LEU	3.2
3	F	412	MET	3.2
1	A	25	SER	3.2
4	G	49	SER	3.2
3	F	394	GLU	3.2
3	C	461	GLU	3.2
1	A	177	LEU	3.2
3	F	436	LEU	3.2
3	C	454	GLU	3.2
3	F	481	VAL	3.2
3	C	395	ASP	3.1
1	A	196	VAL	3.1
3	F	362	GLU	3.1
3	C	453	TYR	3.1
3	F	453	TYR	3.1
3	F	330	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	165	GLU	3.1
4	X	23	SER	3.1
3	C	388	ILE	3.1
3	F	345	GLU	3.1
3	F	395	ASP	3.1
3	F	337	GLY	3.0
2	E	190	LYS	3.0
3	F	457	PRO	3.0
1	A	36	PHE	3.0
3	C	437	GLN	3.0
1	A	3	THR	3.0
1	A	192	GLY	3.0
3	F	341	LYS	3.0
3	C	449	ASP	3.0
3	C	456	SER	3.0
4	G	48	PRO	3.0
3	F	357	GLY	3.0
3	F	355	LYS	2.9
2	B	752	ILE	2.9
4	G	29	TYR	2.9
3	C	412	MET	2.9
3	C	475	THR	2.9
3	C	389	ASN	2.9
3	C	415	GLY	2.9
1	A	13	ILE	2.9
2	E	644	ILE	2.8
3	F	382	LYS	2.8
1	D	127	LEU	2.8
1	A	21	MET	2.8
3	F	186	GLU	2.8
3	F	390	SER	2.8
3	C	343	ASP	2.8
3	F	446	ASP	2.8
3	F	366	HIS	2.8
3	F	367	VAL	2.7
1	D	189	VAL	2.7
3	C	401	ILE	2.7
2	B	650	PRO	2.7
3	C	326	ARG	2.7
3	F	368	ARG	2.7
3	C	472	SER	2.6
1	A	106	TYR	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	137	GLU	2.6
2	E	645	THR	2.6
2	E	189	LYS	2.6
1	D	137	GLU	2.6
3	C	374	GLY	2.6
3	F	371	GLU	2.6
3	C	479	VAL	2.5
3	F	392	LYS	2.5
2	B	671	ARG	2.5
3	F	411	ARG	2.5
1	A	79	VAL	2.5
2	B	647	ALA	2.5
2	B	651	VAL	2.5
3	C	364	GLU	2.5
3	C	371	GLU	2.5
1	A	4	PHE	2.5
1	D	164	GLU	2.5
3	C	375	ILE	2.5
4	X	24	PRO	2.4
1	A	300	LYS	2.4
2	B	648	HIS	2.4
1	D	198	LYS	2.4
3	F	377	LYS	2.4
2	B	646	PRO	2.4
3	C	344	GLU	2.4
3	C	408	GLN	2.4
2	E	649	GLY	2.4
2	B	637	GLU	2.4
3	F	401	ILE	2.4
3	F	479	VAL	2.4
2	B	753	GLY	2.3
3	C	380	LYS	2.3
1	A	123	ILE	2.3
2	B	645	THR	2.3
1	A	69	LYS	2.3
3	C	361	GLY	2.3
1	A	61	TYR	2.3
3	F	558	LEU	2.3
3	C	463	HIS	2.3
3	C	40	ARG	2.2
3	C	465	ILE	2.2
2	B	135	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	162	LEU	2.2
1	D	183	LEU	2.2
3	C	450	GLN	2.2
3	F	350	ASN	2.2
2	B	649	GLY	2.2
3	C	195	LEU	2.2
1	D	197	GLU	2.2
1	D	150	TYR	2.2
3	C	402	LEU	2.2
3	C	411	ARG	2.2
3	F	725	LYS	2.2
1	A	9	PHE	2.2
3	C	382	LYS	2.1
3	F	325	GLN	2.1
3	C	367	VAL	2.1
1	A	183	LEU	2.1
1	A	30	LEU	2.1
1	A	29	GLU	2.1
1	A	179	ALA	2.1
1	A	7	ARG	2.1
1	D	14	ILE	2.1
3	F	496	LYS	2.1
3	C	721	LYS	2.1
3	C	376	LEU	2.1
1	A	161	SER	2.1
4	Y	24	PRO	2.0
2	B	636	ILE	2.0
3	C	327	PHE	2.0
1	A	384	GLU	2.0
3	C	331	GLU	2.0
1	A	38	ILE	2.0
3	C	332	LEU	2.0
3	F	303	ILE	2.0
3	F	304	ASP	2.0
2	E	188	LYS	2.0
2	E	636	ILE	2.0
3	C	381	MET	2.0

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

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SEP	G	47	10/11	0.70	0.27	124,135,140,141	0
4	SEP	Y	26	10/11	0.82	0.22	79,84,91,92	0
4	SEP	X	26	10/11	0.87	0.17	79,83,87,89	0
4	SEP	G	40	10/11	0.93	0.11	64,67,72,72	0
4	SEP	I	40	10/11	0.93	0.12	65,71,84,84	0
4	SEP	I	33	10/11	0.96	0.09	55,58,61,62	0
4	SEP	G	33	10/11	0.96	0.11	49,53,54,55	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.