



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:25 AM EDT

PDB ID : 7Z42 / pdb_00007z42
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

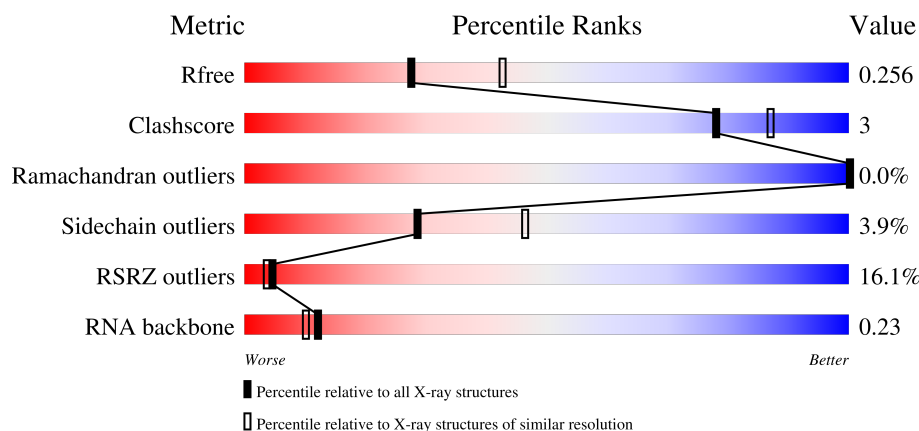
1 Overall quality at a glance

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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)
RNA backbone	3983	1058 (2.70-2.14)

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 ≥ 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	17% 86% 9% ••
1	D	751	13% 85% 9% 5%
2	B	772	8% 88% 9% ••
2	E	772	4% 86% 10% ••

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Mol	Chain	Length	Quality of chain
3	C	798	23% 82% 8% 10%
3	F	798	24% 82% 8% 9%
4	G	28	21% 75% 25%
4	I	28	11% 64% 36%
4	X	28	11% 14% 86%
4	Y	28	7% 7% 89%
5	H	13	62% 31% 8%
5	V	13	62% 38%

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
1	A	721	Total	C	N	O	S	0	1	0
			5787	3675	970	1101	41			
1	D	715	Total	C	N	O	S	0	1	0
			5750	3652	962	1095	41			

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
2	B	754	Total	C	N	O	S	0	0	0
			5911	3731	1024	1104	52			
2	E	743	Total	C	N	O	S	0	0	0
			5818	3671	1004	1091	52			

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
3	C	718	Total	C	N	O	S	0	0	0
			5746	3654	1001	1051	40			
3	F	728	Total	C	N	O	S	0	1	0
			5838	3712	1023	1063	40			

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			

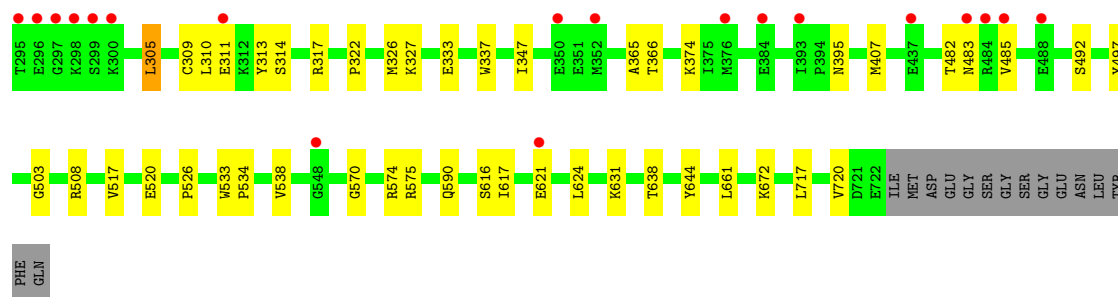
- Molecule 6 is water.

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

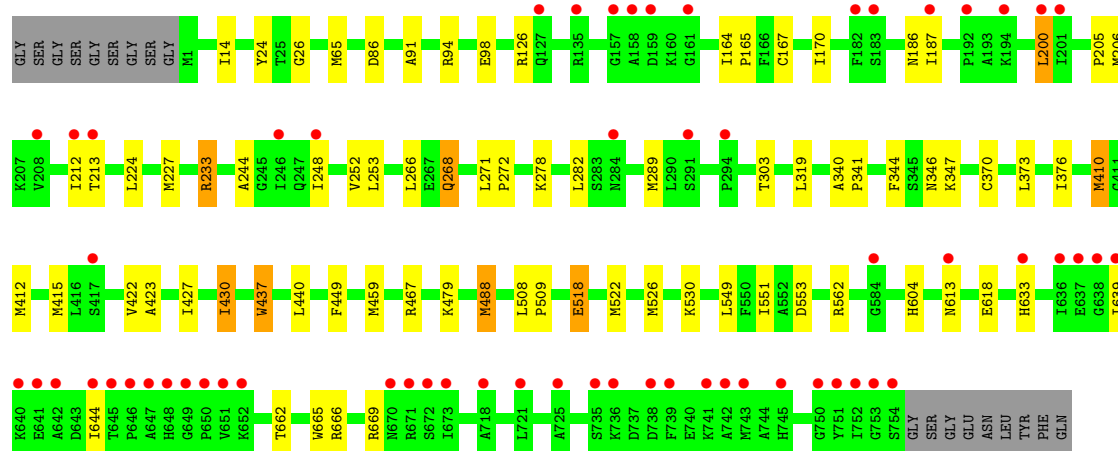
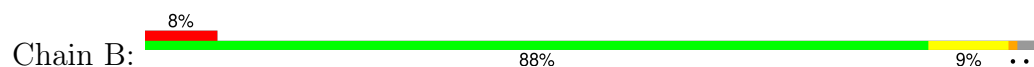
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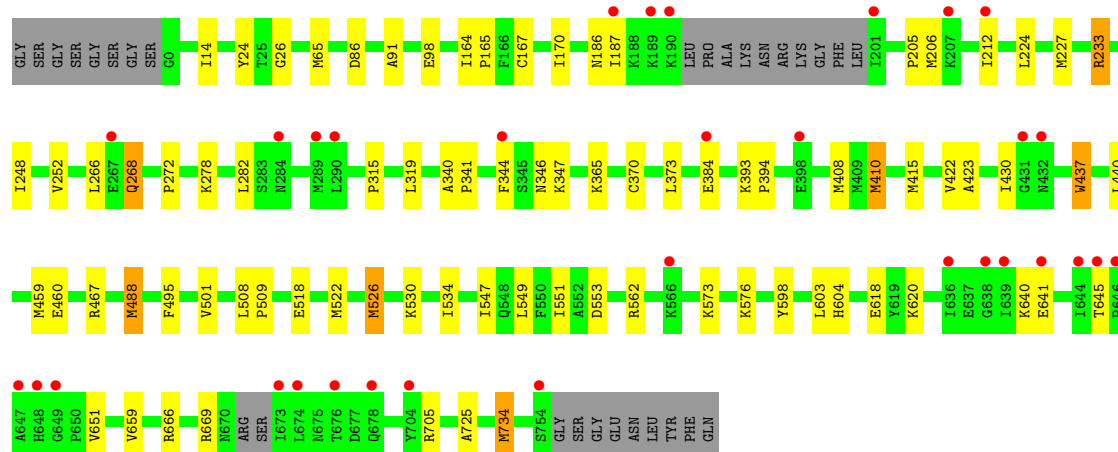
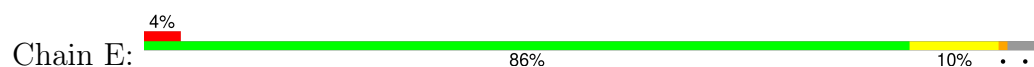
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	30	Total 30	O 30	0	0
6	C	20	Total 20	O 20	0	0
6	D	39	Total 39	O 39	0	0
6	E	43	Total 43	O 43	0	0
6	F	16	Total 16	O 16	0	0
6	G	1	Total 1	O 1	0	0
6	H	6	Total 6	O 6	0	0
6	I	1	Total 1	O 1	0	0
6	V	7	Total 7	O 7	0	0



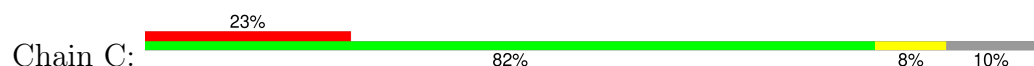
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



• Molecule 2: RNA-directed RNA polymerase catalytic subunit



• Molecule 3: Polymerase basic protein 2



SER ASN ASP ILE SER GLN GLY ILE LYS ARG GLN ARG MET THR VAL GLU SER MET GLY TRP ALA SER LEU SER GLY TRP SER HIS PRO PHE GLU LYS GLY SER GLY SER GLU ASN LEU TYR PHE GLN

- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain Y:  7% 89%

TYR SER P24 T25 S26 PRO SER TYR SER PRO ARG THR SEP PRO MET THR VAL GLU SER MET THR SEP PRO ALA SER LEU SER GLY TRP SER HIS PRO PHE GLU LYS GLY SER GLY SER GLU ASN LEU TYR PHE GLN

- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain G:  21% 75% 25%

Y29 T39 Y43 T46 S47 P48 S49 TYR SER PRO THR SEP PRO SER

- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain X:  11% 14% 86%

TYR S23 P24 T25 S26 PRO SER TYR SER PRO ARG THR SEP PRO MET THR VAL GLU SER MET THR SEP PRO ALA SER LEU SER GLY TRP SER HIS PRO PHE GLU LYS GLY SER GLY SER GLU ASN LEU TYR PHE GLN

- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain I:  11% 64% 36%

Y29 T39 T46 SEP PRO PRO SER TYR SER PRO ARG THR SEP PRO SER

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

Chain H:  62% 31% 8%

A1 A4 G5 U6 A7 A11 G12 A13

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

Chain V:  62% 38%

A1 A4 G5 U6 A7 A11 G12 A13

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.42Å)	Xtriage
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 (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	35949	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.02	0/5903	1.47	2/7959 (0.0%)
1	D	1.02	0/5866	1.47	2/7910 (0.0%)
2	B	1.03	0/6028	1.48	4/8127 (0.0%)
2	E	1.03	0/5931	1.48	2/7995 (0.0%)
3	C	1.04	0/5844	1.44	1/7852 (0.0%)
3	F	1.03	0/5939	1.44	1/7982 (0.0%)
4	G	0.81	0/140	1.04	0/189
4	I	0.88	0/127	1.09	0/173
4	X	0.94	0/20	1.13	0/27
4	Y	0.65	0/14	1.17	0/18
5	H	0.76	0/298	1.06	2/462 (0.4%)
5	V	0.76	0/298	1.04	1/462 (0.2%)
All	All	1.02	0/36408	1.45	15/49156 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	5	G	P-O3'-C3'	-5.77	111.54	120.20
5	H	12	G	P-O3'-C3'	-5.51	111.93	120.20
3	C	361	GLY	CA-C-O	-5.49	118.44	122.23
2	E	553	ASP	CA-C-N	5.44	127.51	120.44
2	E	553	ASP	C-N-CA	5.44	127.51	120.44
3	F	361	GLY	CA-C-O	-5.42	118.49	122.23
2	B	553	ASP	CA-C-N	5.40	127.46	120.44
2	B	553	ASP	C-N-CA	5.40	127.46	120.44
1	A	7	ARG	CA-C-N	5.20	127.51	120.44
1	A	7	ARG	C-N-CA	5.20	127.51	120.44
5	H	5	G	P-O3'-C3'	-5.17	112.45	120.20
1	D	313	TYR	CA-C-N	5.05	127.31	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	TYR	C-N-CA	5.05	127.31	120.38
2	B	303	THR	CA-C-N	5.00	126.42	121.57
2	B	303	THR	C-N-CA	5.00	126.42	121.57

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	5787	0	5761	43	0
1	D	5750	0	5717	37	0
2	B	5911	0	5932	40	0
2	E	5818	0	5824	48	0
3	C	5746	0	5909	26	0
3	F	5838	0	6007	35	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	200	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 3.

All (200) 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:672:LYS:HG3	2:B:488:MET:HE3	1.59	0.84
1:D:83:MET:HE1	1:D:91:VAL:HG21	1.64	0.78
1:D:254:PRO:HB3	2:E:459:MET:HE2	1.68	0.76
1:A:83:MET:HE1	1:A:91:VAL:HG21	1.67	0.75
1:D:80:ILE:HA	1:D:83:MET:HE2	1.70	0.73
1:A:80:ILE:HA	1:A:83:MET:HE2	1.69	0.72
1:A:254:PRO:HB3	2:B:459:MET:HE2	1.73	0.71
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
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
2:E:344:PHE:CD1	2:E:410:MET:HE3	2.37	0.60
1:D:83:MET:HE3	1:D:88:ALA:HA	1.83	0.60
3:F:609:VAL:HA	3:F:688:ARG:HD3	1.84	0.59
1:A:83:MET:HE3	1:A:88:ALA:HA	1.83	0.59
1:D:672:LYS:HG3	2:E:488:MET:HE3	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: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
1:A:294:MET:H	1:A:294:MET:HE3	1.72	0.54
1:A:664:LEU:HD12	1:A:682:MET:HE1	1.89	0.54
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:E:272:PRO:HB3	2:E:415:MET:HE1	1.88	0.54
1:A:226:MET:HE1	2:B:319:LEU:CD2	2.38	0.53
1:D:226:MET:HE1	2:E:319:LEU:CD2	2.38	0.53
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:244:ALA:HB3	2:B:412:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:344:PHE:CE1	2:E:410:MET:HE3	2.45	0.52
2:B:224:LEU:HD13	2:B:410:MET:HG3	1.92	0.52
2:B:522:MET:HE1	2:B:551:ILE:HD11	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
2:E:526:MET:HE3	2:E:603:LEU:HD22	1.92	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
1:A:407:MET:HE1	1:A:638:THR:HB	1.94	0.50
1:A:305:LEU:C	1:A:305:LEU:HD12	2.37	0.50
2:B:187:ILE:CG1	2:B:206:MET:HE2	2.42	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
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:B:187:ILE:HG13	2:B:206:MET:HE2	1.95	0.48
2:E:91:ALA:HB1	2:E:423:ALA:HB1	1.96	0.48
2:E:522:MET:HE3	2:E:598:TYR:CD2	2.49	0.48
1:D:305:LEU:C	1:D:305:LEU:HD12	2.38	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:HE2	1.96	0.48
1:D:181:LEU:HD13	1:D:190:LEU:HD22	1.96	0.48
1:D:407:MET:HE1	1:D:638:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:246:MET:HE3	2:B:467:ARG:HB3	1.96	0.47
1:A:413:LEU:HD12	4:Y:26:SEP:HB3	1.96	0.47
1:D:216:VAL:HG12	1:D:226:MET:HE2	1.96	0.47
2:E:370:CYS:HA	2:E:373:LEU:HD13	1.96	0.47
2:E:522:MET:HE1	2:E:551:ILE:HD11	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
2:E:65:MET:HE1	2:E:346:ASN:HA	1.96	0.47
1:A:216:VAL:HG12	1:A:226:MET:HE2	1.96	0.46
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
1:A:594:ILE:HG12	3:C:675:MET:HE3	1.97	0.46
2:B:272:PRO:HB3	2:B:415:MET:HE1	1.98	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
2:B:344:PHE:CE1	2:B:410:MET:HE3	2.50	0.46
3:F:551:TYR:HB3	3:F:670:ILE:HD13	1.98	0.46
2:B:65:MET:HE1	2:B:346:ASN:HA	1.97	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:D:246:MET:HE1	2:E:467:ARG:HB3	1.99	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
2:E:725:ALA:HA	2:E:734:MET:HE2	2.00	0.44
1:A:682:MET:HG3	2:B:479:LYS:O	2.17	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:MET:HE1	1:A:91:VAL:CG2	2.44	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:E:526:MET:HE1	2:E:547:ILE:HG12	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
2:E:522:MET:HE3	2:E:598:TYR:CE2	2.54	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
1:D:83:MET:HE1	1:D:91:VAL:CG2	2.43	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:285:ILE:O	3:F:289:THR:HG23	2.20	0.41
2:B:437:TRP:C	2:B:437:TRP:CD1	2.99	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
2:E:526:MET:HE3	2:E:603:LEU:CD2	2.51	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
2:E:437:TRP:CD1	2:E:437:TRP:C	2.98	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
3:F:404:MET:HE1	3:F:476: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
3:F:388:ILE:HD12	3:F:396:MET:HE2	2.03	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
1:D:26:GLU:HG2	1:D:34:MET:HE1	2.03	0.41
2:E:187:ILE:HD11	2:E:206:MET:HE3	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
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%)	48	63
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%)	48	63
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%)	620 (97%)	21 (3%)	33	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	638/664 (96%)	612 (96%)	26 (4%)	27	44
2	B	646/657 (98%)	618 (96%)	28 (4%)	26	42
2	E	636/657 (97%)	614 (96%)	22 (4%)	32	51
3	C	628/694 (90%)	602 (96%)	26 (4%)	27	44
3	F	637/694 (92%)	611 (96%)	26 (4%)	27	44
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%)	28	46

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

Mol	Chain	Res	Type
1	A	26	GLU
1	A	51	MET
1	A	141	ASN
1	A	226	MET
1	A	233	ILE
1	A	294	MET
1	A	305	LEU
1	A	319	GLN
1	A	326	MET
1	A	333	GLU
1	A	347	ILE
1	A	376	MET
1	A	384	GLU
1	A	395	ASN
1	A	477	LYS
1	A	485	VAL
1	A	492	SER
1	A	520	GLU
1	A	577	LEU
1	A	617	ILE
1	A	631	LYS
2	B	14	ILE
2	B	94	ARG
2	B	98	GLU
2	B	126	ARG

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Mol	Chain	Res	Type
2	B	200	LEU
2	B	212	ILE
2	B	213	THR
2	B	227	MET
2	B	233	ARG
2	B	253	LEU
2	B	268	GLN
2	B	271	LEU
2	B	376	ILE
2	B	410	MET
2	B	427	ILE
2	B	430	ILE
2	B	437	TRP
2	B	488	MET
2	B	518	GLU
2	B	526	MET
2	B	562	ARG
2	B	613	ASN
2	B	618	GLU
2	B	633	HIS
2	B	639	ILE
2	B	644	ILE
2	B	666	ARG
2	B	669	ARG
3	C	24	GLN
3	C	34	ARG
3	C	226	THR
3	C	243	ARG
3	C	251	ASN
3	C	273	ILE
3	C	274	VAL
3	C	289	THR
3	C	324	ARG
3	C	332	LEU
3	C	378	LYS
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

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Mol	Chain	Res	Type
3	C	601	LEU
3	C	631	ASN
3	C	647	GLU
3	C	689	SER
3	C	694	VAL
3	C	728	ILE
3	C	732	GLN
3	C	737	LYS
1	D	26	GLU
1	D	30	LEU
1	D	40	VAL
1	D	43	GLU
1	D	141	ASN
1	D	226	MET
1	D	233	ILE
1	D	243	LEU
1	D	251	SER
1	D	255	LYS
1	D	263	ARG
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	347	ILE
1	D	395	ASN
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	98	GLU
2	E	212	ILE
2	E	227	MET
2	E	233	ARG
2	E	268	GLN
2	E	384	GLU
2	E	410	MET

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Mol	Chain	Res	Type
2	E	430	ILE
2	E	437	TRP
2	E	460	GLU
2	E	488	MET
2	E	518	GLU
2	E	526	MET
2	E	562	ARG
2	E	576	LYS
2	E	618	GLU
2	E	620	LYS
2	E	666	ARG
2	E	669	ARG
2	E	705	ARG
2	E	734	MET
3	F	34	ARG
3	F	125	MET
3	F	226	THR
3	F	273	ILE
3	F	274	VAL
3	F	289	THR
3	F	324	ARG
3	F	332	LEU
3	F	340	PHE
3	F	372	CYS
3	F	378	LYS
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	607	GLN
3	F	624	SER
3	F	647	GLU
3	F	689	SER
3	F	694	VAL
3	F	732	GLN
3	F	737	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	71	GLN
1	A	152	GLN
1	A	293	ASN
1	A	319	GLN
1	A	433	HIS
1	A	467	ASN
1	A	470	ASN
1	A	620	GLN
2	B	137	GLN
2	B	144	ASN
2	B	536	ASN
2	B	613	ASN
3	C	549	ASN
1	D	52	ASN
1	D	152	GLN
1	D	433	HIS
1	D	590	GLN
2	E	127	GLN
2	E	310	ASN
2	E	536	ASN
2	E	670	ASN
2	E	675	ASN
2	E	710	GLN
3	F	16	ASN
3	F	37	ASN
3	F	424	ASN
3	F	437	GLN

5.3.3 RNA ⓘ

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

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Mol	Chain	Res	Type
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 ⓘ

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	40	4	8,9,10	0.74	0	7,12,14	0.57	0
4	SEP	G	47	4	8,9,10	0.56	0	7,12,14	0.66	0
4	SEP	G	33	4	8,9,10	0.58	0	7,12,14	0.67	0
4	SEP	I	40	4	8,9,10	0.53	0	7,12,14	0.66	0
4	SEP	Y	26	4	8,9,10	0.59	0	7,12,14	0.67	0
4	SEP	X	26	4	8,9,10	0.57	0	7,12,14	0.71	0
4	SEP	I	33	4	8,9,10	0.58	0	7,12,14	0.64	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	40	4	-	4/6/8/10	-
4	SEP	G	47	4	-	2/6/8/10	-
4	SEP	G	33	4	-	3/6/8/10	-
4	SEP	I	40	4	-	0/6/8/10	-
4	SEP	Y	26	4	-	2/6/8/10	-
4	SEP	X	26	4	-	1/6/8/10	-
4	SEP	I	33	4	-	3/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	33	SEP	C-CA-CB-OG
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	I	33	SEP	C-CA-CB-OG
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
4	Y	26	SEP	C-CA-CB-OG

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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	721/751 (96%)	0.82	131 (18%) 3 3	21, 40, 126, 149	1 (0%)
1	D	715/751 (95%)	0.74	101 (14%) 6 5	21, 39, 116, 139	1 (0%)
2	B	754/772 (97%)	0.61	61 (8%) 18 14	23, 45, 76, 116	0
2	E	743/772 (96%)	0.42	32 (4%) 40 35	23, 42, 69, 110	0
3	C	718/798 (89%)	1.42	185 (25%) 1 1	25, 56, 185, 226	0
3	F	728/798 (91%)	1.32	193 (26%) 1 1	17, 54, 172, 193	1 (0%)
4	G	18/28 (64%)	1.59	6 (33%) 1 1	46, 68, 131, 137	0
4	I	16/28 (57%)	1.33	3 (18%) 3 2	46, 63, 75, 89	0
4	X	3/28 (10%)	3.51	3 (100%) 0 0	94, 94, 96, 97	0
4	Y	2/28 (7%)	4.82	2 (100%) 0 0	98, 98, 98, 98	0
5	H	13/13 (100%)	-0.64	0 100 100	25, 29, 56, 69	0
5	V	13/13 (100%)	-0.88	0 100 100	25, 28, 40, 47	0
All	All	4444/4780 (92%)	0.88	717 (16%) 4 4	17, 46, 139, 226	3 (0%)

All (717) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	358	ILE	7.6
3	F	423	LEU	7.5
3	C	356	ILE	7.3
3	F	358	ILE	6.9
3	C	387	LEU	6.8
3	F	386	LEU	6.8
3	F	427	GLY	6.6
3	F	429	LEU	6.6
3	F	426	ALA	6.5
2	E	647	ALA	6.5
3	F	375	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
3	F	428	GLN	6.3
3	F	441	LEU	6.3
3	F	340	PHE	6.2
3	F	459	ALA	6.1
3	C	386	LEU	6.0
3	F	387	LEU	6.0
3	C	448	PHE	5.9
2	E	645	THR	5.9
3	C	441	LEU	5.9
1	A	201	ASP	5.9
3	F	425	ARG	5.9
3	C	400	ILE	5.8
3	C	432	PRO	5.8
3	C	399	LEU	5.7
3	F	430	LEU	5.7
3	C	346	ILE	5.7
3	C	375	ILE	5.7
1	A	30	LEU	5.6
3	C	340	PHE	5.6
3	F	347	LEU	5.6
3	C	431	SER	5.5
3	F	440	PHE	5.5
3	C	420	ILE	5.5
3	C	416	VAL	5.4
3	C	480	VAL	5.4
3	C	406	PHE	5.4
3	F	420	ILE	5.4
2	E	673	ILE	5.3
3	C	1	MET	5.3
3	C	447	LEU	5.2
4	X	25	THR	5.2
1	A	196	VAL	5.2
4	Y	25	THR	5.2
3	C	440	PHE	5.2
3	F	88	THR	5.2
3	F	481	VAL	5.1
1	A	33	ALA	5.1
2	B	752	ILE	5.1
3	F	86	ILE	5.1
1	A	6	THR	5.1
3	C	459	ALA	5.1
3	C	587	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
2	E	644	ILE	5.0
3	C	361	GLY	5.0
3	F	469	MET	5.0
3	C	354	GLN	5.0
3	F	431	SER	4.9
3	C	401	ILE	4.9
1	D	186	LEU	4.9
2	E	648	HIS	4.9
3	F	402	LEU	4.9
3	F	479	VAL	4.8
3	F	424	ASN	4.8
1	D	299	SER	4.8
2	B	646	PRO	4.8
3	C	413	PHE	4.8
3	C	462	LEU	4.8
3	F	447	LEU	4.8
3	F	482	THR	4.8
3	C	468	SER	4.8
3	F	383	LEU	4.8
1	A	192	GLY	4.7
3	F	353	ILE	4.7
3	C	385	LYS	4.7
3	C	476	LEU	4.7
3	C	359	TRP	4.7
3	C	341	LYS	4.7
3	C	418	GLY	4.7
2	E	646	PRO	4.7
3	F	403	CYS	4.7
3	F	462	LEU	4.7
3	F	354	GLN	4.6
2	B	651	VAL	4.6
3	F	400	ILE	4.6
3	C	347	LEU	4.6
3	C	457	PRO	4.6
3	F	451	TRP	4.6
3	C	434	TYR	4.5
3	C	474	TYR	4.5
3	F	433	MET	4.5
3	F	410	THR	4.5
3	C	357	GLY	4.5
3	F	480	VAL	4.5
3	C	433	MET	4.5

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Mol	Chain	Res	Type	RSRZ
3	C	360	ASP	4.5
3	F	434	TYR	4.5
2	B	645	THR	4.5
3	C	410	THR	4.5
3	C	436	LEU	4.5
2	B	649	GLY	4.4
3	F	465	ILE	4.4
4	Y	24	PRO	4.4
2	B	754	SER	4.4
3	F	471	ALA	4.4
2	E	201	ILE	4.4
3	C	86	ILE	4.4
3	C	439	TYR	4.4
3	F	406	PHE	4.4
1	A	186	LEU	4.4
3	C	352	THR	4.3
3	F	453	TYR	4.3
2	B	641	GLU	4.3
3	C	442	ASN	4.3
3	C	451	TRP	4.3
3	F	87	GLY	4.3
3	F	352	THR	4.3
3	F	176	ILE	4.3
2	B	650	PRO	4.2
3	F	432	PRO	4.2
1	A	13	ILE	4.2
2	B	735	SER	4.2
1	A	189	VAL	4.2
3	C	404	MET	4.2
3	F	439	TYR	4.2
3	C	353	ILE	4.2
3	F	474	TYR	4.1
3	F	388	ILE	4.1
1	D	127	LEU	4.1
3	F	186	GLU	4.1
1	A	191	ILE	4.1
3	F	401	ILE	4.1
3	F	422	PHE	4.1
3	F	442	ASN	4.1
2	B	751	TYR	4.1
1	D	296	GLU	4.0
2	B	640	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	THR	4.0
3	F	404	MET	4.0
3	C	471	ALA	4.0
1	A	156	LEU	4.0
3	C	383	LEU	4.0
3	F	336	SER	4.0
3	F	396	MET	4.0
1	A	183	LEU	4.0
3	C	389	ASN	3.9
1	A	64	LEU	3.9
3	C	479	VAL	3.9
4	G	48	PRO	3.9
3	C	465	ILE	3.9
1	D	162	LEU	3.9
1	A	25	SER	3.9
3	F	181	THR	3.9
3	C	405	VAL	3.9
3	F	413	PHE	3.9
3	F	436	LEU	3.9
1	A	131	TYR	3.8
3	C	381	MET	3.8
3	C	453	TYR	3.8
3	F	83	ALA	3.8
4	I	29	TYR	3.8
3	F	326	ARG	3.8
3	C	419	GLU	3.8
3	F	384	GLU	3.8
3	C	482	THR	3.8
3	C	388	ILE	3.8
3	C	327	PHE	3.8
1	A	311	GLU	3.8
3	F	421	ASN	3.8
1	D	139	LEU	3.8
3	F	351	GLY	3.7
1	A	123	ILE	3.7
3	F	437	GLN	3.7
3	F	452	GLY	3.7
3	F	346	ILE	3.7
1	A	51	MET	3.7
3	C	469	MET	3.7
3	F	349	GLY	3.7
1	A	127	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	458	LYS	3.7
3	C	351	GLY	3.7
3	C	195	LEU	3.7
3	F	476	LEU	3.7
3	F	405	VAL	3.6
3	F	174	ALA	3.6
1	D	300	LYS	3.6
3	C	326	ARG	3.6
3	F	416	VAL	3.6
1	A	142	SER	3.6
2	E	649	GLY	3.6
3	C	8	LEU	3.6
2	E	566	LYS	3.6
3	C	481	VAL	3.6
1	D	161	SER	3.6
2	E	754	SER	3.6
2	B	671	ARG	3.6
1	A	35	LEU	3.6
3	C	83	ALA	3.6
3	F	399	LEU	3.6
3	C	41	ILE	3.6
1	A	384	GLU	3.5
3	C	344	GLU	3.5
3	F	359	TRP	3.5
3	F	407	SER	3.5
1	D	168	GLY	3.5
1	A	63	ALA	3.5
3	C	376	LEU	3.5
3	C	463	HIS	3.5
3	C	458	LYS	3.5
1	D	196	VAL	3.5
3	F	348	ILE	3.5
3	F	372	CYS	3.5
2	B	736	LYS	3.5
3	C	739	VAL	3.4
3	F	435	GLN	3.4
3	F	464	GLY	3.4
1	D	160	SER	3.4
3	F	362	GLU	3.4
3	F	738	VAL	3.4
1	D	60	ALA	3.4
3	C	478	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	460	SER	3.4
1	D	133	TRP	3.4
3	C	740	LYS	3.4
3	F	385	LYS	3.4
2	B	753	GLY	3.4
1	A	1	MET	3.3
1	A	150	TYR	3.3
3	C	372	CYS	3.3
3	F	361	GLY	3.3
1	A	22	ALA	3.3
1	D	30	LEU	3.3
3	F	356	ILE	3.3
2	E	190	LYS	3.3
3	F	341	LYS	3.3
3	C	342	ASN	3.3
3	F	376	LEU	3.3
3	C	87	GLY	3.3
1	D	5	ILE	3.3
2	B	672	SER	3.3
1	A	154	TYR	3.3
1	A	42	LEU	3.3
1	A	177	LEU	3.3
1	A	132	PHE	3.2
3	C	443	ARG	3.2
3	C	402	LEU	3.2
1	A	79	VAL	3.2
3	F	328	GLY	3.2
1	A	161	SER	3.2
3	F	159	ASP	3.2
3	F	158	PRO	3.2
3	C	393	LYS	3.2
3	C	477	LYS	3.2
3	C	176	ILE	3.2
1	A	31	GLN	3.2
3	C	407	SER	3.2
3	C	343	ASP	3.2
3	F	207	TYR	3.2
3	C	349	GLY	3.2
3	C	697	GLY	3.2
3	F	478	GLY	3.2
2	B	644	ILE	3.2
3	C	728	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	132	PHE	3.2
1	D	148	PHE	3.2
3	C	680	LYS	3.2
3	F	1	MET	3.2
1	D	191	ILE	3.2
2	B	187	ILE	3.2
3	F	391	ALA	3.1
3	F	438	ARG	3.1
3	F	382	LYS	3.1
1	A	32	PRO	3.1
3	C	199	MET	3.1
2	E	432	ASN	3.1
3	F	370	GLY	3.1
1	A	184	LYS	3.1
1	A	187	TRP	3.1
1	A	352	MET	3.1
3	F	182	TRP	3.1
3	F	460	SER	3.1
1	A	73	LEU	3.1
3	C	332	LEU	3.1
1	A	387	CYS	3.1
1	A	36	PHE	3.1
3	F	332	LEU	3.1
3	F	398	ASP	3.1
3	F	409	ASP	3.1
3	F	448	PHE	3.1
1	A	299	SER	3.1
1	D	157	SER	3.1
1	A	20	THR	3.0
3	C	437	GLN	3.0
3	F	380	LYS	3.0
4	G	29	TYR	3.0
3	F	365	PHE	3.0
3	F	355	LYS	3.0
1	A	12	THR	3.0
1	A	54	LEU	3.0
1	A	190	LEU	3.0
3	F	389	ASN	3.0
3	C	452	GLY	3.0
3	F	418	GLY	3.0
1	A	5	ILE	3.0
1	A	200	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	325	GLN	3.0
3	F	408	GLN	3.0
1	D	1	MET	3.0
1	D	156	LEU	3.0
3	C	403	CYS	3.0
1	A	102	GLU	2.9
3	F	726	ALA	2.9
1	A	139	LEU	2.9
1	A	300	LYS	2.9
3	C	355	LYS	2.9
3	C	377	LYS	2.9
1	A	24	PHE	2.9
3	F	304	ASP	2.9
3	F	463	HIS	2.9
4	G	46	THR	2.9
1	A	106	TYR	2.9
1	A	148	PHE	2.9
1	A	66	GLY	2.9
2	B	750	GLY	2.9
3	C	412	MET	2.9
3	C	415	GLY	2.9
3	F	337	GLY	2.9
3	F	412	MET	2.9
4	I	39	THR	2.9
1	A	69	LYS	2.9
1	D	136	LYS	2.9
3	F	89	LYS	2.9
1	A	133	TRP	2.9
1	D	166	GLY	2.9
2	B	636	ILE	2.9
3	C	183	ILE	2.9
2	B	741	LYS	2.9
3	F	496	LYS	2.9
1	A	28	PRO	2.9
3	C	534	THR	2.9
3	F	330	LEU	2.9
3	F	360	ASP	2.9
1	A	61	TYR	2.9
1	A	152	GLN	2.9
1	D	106	TYR	2.9
1	D	126	GLY	2.9
2	B	584	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	638	GLY	2.9
1	A	157	SER	2.8
1	A	395	ASN	2.8
2	E	636	ILE	2.8
1	D	190	LEU	2.8
3	C	450	GLN	2.8
2	B	637	GLU	2.8
2	E	267	GLU	2.8
1	A	7	ARG	2.8
3	F	415	GLY	2.8
1	A	393	ILE	2.8
2	B	639	ILE	2.8
3	C	390	SER	2.8
3	F	342	ASN	2.8
1	A	44	VAL	2.8
3	F	457	PRO	2.8
1	D	376	MET	2.8
1	A	16	LYS	2.8
1	A	138	LYS	2.8
2	B	633	HIS	2.8
2	B	648	HIS	2.8
3	C	207	TYR	2.8
1	D	172	SER	2.8
3	F	180	SER	2.8
1	D	189	VAL	2.8
2	B	647	ALA	2.8
1	D	29	GLU	2.8
3	C	380	LYS	2.8
3	C	414	GLN	2.8
3	F	393	LYS	2.8
3	F	397	ARG	2.8
3	C	365	PHE	2.8
1	D	131	TYR	2.8
3	F	183	ILE	2.8
1	A	0	SER	2.8
3	C	81	THR	2.8
1	A	164	GLU	2.8
1	A	298	LYS	2.8
2	B	652	LYS	2.8
3	C	345	GLU	2.8
1	D	140	GLY	2.7
3	C	727	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	291	SER	2.7
1	A	103	THR	2.7
3	C	560	THR	2.7
3	C	396	MET	2.7
3	C	495	GLU	2.7
1	A	39	CYS	2.7
3	C	398	ASP	2.7
2	E	187	ILE	2.7
1	A	172	SER	2.7
1	A	162	LEU	2.7
1	A	134	LYS	2.7
1	A	165	GLU	2.7
3	C	362	GLU	2.7
3	C	325	GLN	2.7
1	A	140	GLY	2.7
4	X	24	PRO	2.7
1	A	105	LYS	2.7
3	C	254	THR	2.7
3	C	438	ARG	2.7
1	D	164	GLU	2.7
3	F	473	ASP	2.7
3	F	335	ILE	2.7
1	A	158	ASN	2.7
2	B	670	ASN	2.7
1	A	3	THR	2.7
3	C	182	TRP	2.7
1	D	32	PRO	2.6
1	D	298	LYS	2.6
1	D	483	ASN	2.6
3	C	686	ARG	2.6
3	F	368	ARG	2.6
3	F	390	SER	2.6
1	A	128	ALA	2.6
1	D	150	TYR	2.6
3	F	378	LYS	2.6
3	F	177	PRO	2.6
1	A	171	LEU	2.6
1	D	158	ASN	2.6
2	B	613	ASN	2.6
3	F	631	ASN	2.6
3	F	717	LEU	2.6
4	X	23	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	435	GLN	2.6
3	C	721	LYS	2.6
3	C	177	PRO	2.6
1	A	101	ILE	2.6
1	D	437	GLU	2.6
3	F	467	GLU	2.6
3	F	724	GLU	2.6
3	C	11	GLN	2.6
3	C	180	SER	2.6
1	D	6	THR	2.6
1	D	179	ALA	2.6
2	B	157	GLY	2.6
3	F	339	GLY	2.6
3	F	374	GLY	2.6
3	F	443	ARG	2.6
3	C	682	GLU	2.6
3	F	247[A]	HIS	2.6
3	F	444	SER	2.6
3	F	468	SER	2.6
1	D	61	TYR	2.6
1	D	7	ARG	2.5
1	A	126	GLY	2.5
1	A	4	PHE	2.5
4	I	46	THR	2.5
2	B	135	ARG	2.5
3	C	417	ARG	2.5
1	A	46	TYR	2.5
3	F	704	TYR	2.5
2	E	638	GLY	2.5
1	D	13	ILE	2.5
1	D	144	GLU	2.5
1	D	36	PHE	2.5
1	D	183	LEU	2.5
3	F	327	PHE	2.5
3	F	567	LEU	2.5
1	A	114	LYS	2.5
3	F	350	ASN	2.5
1	D	22	ALA	2.5
4	G	39	THR	2.5
1	D	484	ARG	2.5
1	A	75	PRO	2.5
1	A	68	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	335	ILE	2.5
1	A	202	PHE	2.5
2	B	182	PHE	2.5
1	A	40	VAL	2.5
1	D	128	ALA	2.5
1	D	169	ARG	2.5
3	F	338	ARG	2.5
1	D	3	THR	2.5
1	D	295	THR	2.5
3	F	379	SER	2.5
2	E	384	GLU	2.5
3	F	682	GLU	2.5
2	B	159	ASP	2.5
1	A	10	GLN	2.5
1	A	169	ARG	2.5
3	C	181	THR	2.5
3	C	256	SER	2.5
3	C	328	GLY	2.4
3	F	454	GLU	2.4
3	F	461	GLU	2.4
1	A	119	ILE	2.4
1	A	135	LYS	2.4
1	D	134	LYS	2.4
2	B	246	ILE	2.4
3	C	12	LEU	2.4
1	D	9	PHE	2.4
3	C	470	ASN	2.4
3	F	466	ASN	2.4
1	D	352	MET	2.4
1	A	115	THR	2.4
1	A	350	GLU	2.4
1	D	297	GLY	2.4
2	E	431	GLY	2.4
3	C	556	LYS	2.4
3	F	725	LYS	2.4
2	B	673	ILE	2.4
1	A	77	TYR	2.4
1	D	154	TYR	2.4
3	C	408	GLN	2.4
3	F	558	LEU	2.4
3	F	686	ARG	2.4
3	F	381	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	88	THR	2.4
1	D	116	LYS	2.4
1	D	311	GLU	2.4
3	C	179	GLU	2.4
3	C	467	GLU	2.4
3	F	344	GLU	2.4
1	A	199	GLY	2.4
3	C	644	GLY	2.4
3	C	65	ASP	2.4
1	D	31	GLN	2.4
2	B	745	HIS	2.4
3	F	417	ARG	2.4
2	E	344	PHE	2.4
1	A	146	MET	2.4
1	A	8	ASN	2.4
2	E	284	ASN	2.4
2	B	213	THR	2.4
2	B	294	PRO	2.4
2	E	189	LYS	2.4
3	C	523	GLU	2.4
3	F	81	THR	2.4
3	F	357	GLY	2.4
1	A	14	ILE	2.4
2	B	212	ILE	2.4
1	D	171	LEU	2.4
3	C	446	ASP	2.4
3	F	343	ASP	2.4
1	A	488	GLU	2.4
3	F	345	GLU	2.4
3	F	419	GLU	2.4
3	F	475	THR	2.3
3	F	456	SER	2.3
3	C	723	GLY	2.3
1	A	145	LEU	2.3
1	A	147	ILE	2.3
1	A	188	GLN	2.3
1	D	110	LEU	2.3
2	E	678	GLN	2.3
3	C	449	ASP	2.3
1	D	46	TYR	2.3
3	C	698	PHE	2.3
2	B	642	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	337	GLY	2.3
3	C	370	GLY	2.3
3	C	464	GLY	2.3
1	D	125	LYS	2.3
2	B	194	LYS	2.3
3	F	333	LYS	2.3
3	F	377	LYS	2.3
1	D	0	SER	2.3
4	G	49	SER	2.3
1	D	272	HIS	2.3
3	F	366	HIS	2.3
2	E	212	ILE	2.3
1	D	261	ASP	2.3
3	F	721	LYS	2.3
1	D	350	GLU	2.3
1	D	621	GLU	2.3
2	B	158	ALA	2.3
1	D	548	GLY	2.3
3	F	723	GLY	2.3
3	C	276	SER	2.3
3	C	444	SER	2.3
2	B	743	MET	2.3
3	C	159	ASP	2.3
1	A	57	GLU	2.3
1	D	159	GLU	2.3
2	B	739	PHE	2.3
1	A	185	ASN	2.2
2	B	284	ASN	2.2
1	D	101	ILE	2.2
1	D	145	LEU	2.2
1	D	146	MET	2.2
1	A	321	ASP	2.2
3	F	446	ASP	2.2
1	D	165	GLU	2.2
1	D	194	GLU	2.2
3	F	483	ARG	2.2
2	E	704	TYR	2.2
2	B	127	GLN	2.2
2	E	676	THR	2.2
3	F	11	GLN	2.2
1	A	136	LYS	2.2
1	D	138	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	143	MET	2.2
2	E	207	LYS	2.2
3	F	477	LYS	2.2
3	C	348	ILE	2.2
1	D	130	ASP	2.2
1	A	144	GLU	2.2
3	C	14	ARG	2.2
2	B	161	GLY	2.2
2	E	290	LEU	2.2
3	C	197	GLY	2.2
3	F	681	ILE	2.2
3	F	472	SER	2.2
3	C	473	ASP	2.2
1	D	384	GLU	2.2
2	E	398	GLU	2.2
2	E	641	GLU	2.2
3	C	633	GLU	2.2
1	A	117	ARG	2.2
3	F	373	ARG	2.2
1	D	485	VAL	2.2
3	F	367	VAL	2.2
1	D	114	LYS	2.2
3	C	445	ASN	2.2
1	A	357	GLN	2.2
1	D	35	LEU	2.2
2	B	721	LEU	2.2
3	C	369	CYS	2.2
3	C	374	GLY	2.2
3	C	642	LEU	2.2
3	C	704	TYR	2.2
1	A	129	ASP	2.2
1	A	195	ASP	2.2
3	F	179	GLU	2.2
2	B	192	PRO	2.2
3	C	722	PRO	2.2
1	A	9	PHE	2.2
1	D	184	LYS	2.2
1	A	170	VAL	2.1
1	A	720	VAL	2.1
2	B	208	VAL	2.1
2	B	742	ALA	2.1
1	D	175	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	187	LEU	2.1
3	F	560	THR	2.1
1	D	393	ILE	2.1
2	B	417	SER	2.1
3	C	456	SER	2.1
3	C	158	PRO	2.1
1	D	4	PHE	2.1
2	E	289	MET	2.1
3	F	450	GLN	2.1
1	D	185	ASN	2.1
3	C	350	ASN	2.1
3	C	466	ASN	2.1
1	A	295	THR	2.1
3	C	628	LEU	2.1
3	F	175	GLY	2.1
1	D	233	ILE	2.1
2	E	639	ILE	2.1
3	C	107	ILE	2.1
1	A	29	GLU	2.1
3	C	373	ARG	2.1
1	A	719	SER	2.1
1	D	198	LYS	2.1
3	F	739	VAL	2.1
1	D	33	ALA	2.1
1	D	174	LEU	2.1
2	E	674	LEU	2.1
3	C	3	LEU	2.1
3	C	13	LEU	2.1
3	C	79	LEU	2.1
3	C	279	LEU	2.1
1	A	549	ARG	2.1
3	C	48	ARG	2.1
2	B	248	ILE	2.1
3	C	461	GLU	2.1
4	G	43	TYR	2.1
1	A	112	ASP	2.1
1	D	142	SER	2.1
3	C	157	PRO	2.1
1	A	53	PHE	2.1
1	D	121	VAL	2.1
1	D	187	TRP	2.1
3	C	566	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	720	LEU	2.1
1	A	70	GLU	2.1
3	F	713	THR	2.1
3	F	303	ILE	2.1
3	C	707	ASP	2.1
1	A	155	SER	2.1
3	F	630	SER	2.1
1	D	83	MET	2.1
1	D	10	GLN	2.0
1	A	118	PHE	2.0
1	A	121	VAL	2.0
2	B	718	ALA	2.0
2	B	725	ALA	2.0
3	F	629	ARG	2.0
1	A	107	LEU	2.0
1	A	110	LEU	2.0
3	F	720	LEU	2.0
3	C	112	GLY	2.0
3	F	84	GLU	2.0
1	A	125	LYS	2.0
2	B	201	ILE	2.0
3	F	199	MET	2.0
3	C	184	HIS	2.0
1	D	24	PHE	2.0
3	C	738	VAL	2.0
1	D	488	GLU	2.0
2	B	200	LEU	2.0
3	F	8	LEU	2.0
3	C	382	LYS	2.0
1	D	123	ILE	2.0
2	B	738	ASP	2.0
3	F	707	ASP	2.0
2	B	183	SER	2.0
3	F	498	SER	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, 95th 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($\text{\AA}^2$)	Q<0.9
4	SEP	G	47	10/11	0.36	0.15	124,135,140,141	0
4	SEP	Y	26	10/11	0.78	0.17	79,84,91,92	0
4	SEP	X	26	10/11	0.79	0.14	79,83,87,89	0
4	SEP	G	40	10/11	0.86	0.14	64,67,72,72	0
4	SEP	I	40	10/11	0.88	0.11	65,71,84,84	0
4	SEP	I	33	10/11	0.91	0.10	55,58,61,62	0
4	SEP	G	33	10/11	0.92	0.10	49,53,54,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.