



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:33 AM EDT

PDB ID : 7DKG
Title : Influenza H5N1 nucleoprotein (truncated) in complex with nucleotides
Authors : Tang, Y.S.; Xu, S.; Chen, Y.W.; Wang, J.H.; Shaw, P.C.
Deposited on : 2020-11-24
Resolution : 3.00 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

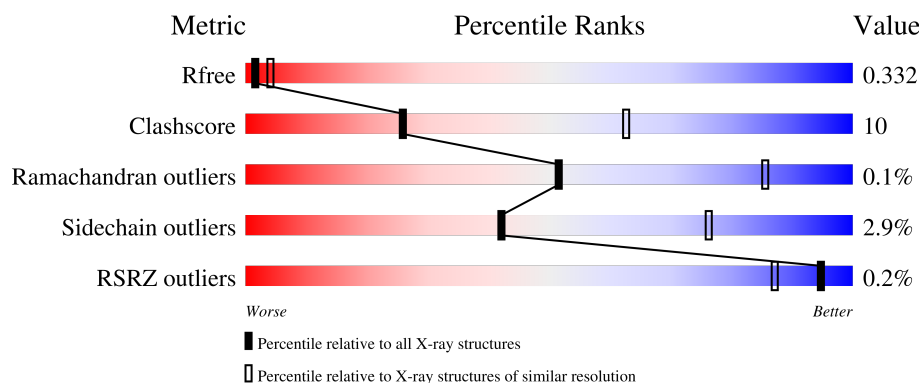
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	505	 63% 14% • 22%
1	B	505	 62% 17% • 19%
2	C	8	 38% 62%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6421 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3104	1927	576	575	26			
1	B	409	Total	C	N	O	S	0	0	0
			3205	1988	595	596	26			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q9PX50
A	-34	GLY	-	expression tag	UNP Q9PX50
A	-33	SER	-	expression tag	UNP Q9PX50
A	-32	SER	-	expression tag	UNP Q9PX50
A	-31	HIS	-	expression tag	UNP Q9PX50
A	-30	HIS	-	expression tag	UNP Q9PX50
A	-29	HIS	-	expression tag	UNP Q9PX50
A	-28	HIS	-	expression tag	UNP Q9PX50
A	-27	HIS	-	expression tag	UNP Q9PX50
A	-26	HIS	-	expression tag	UNP Q9PX50
A	-25	SER	-	expression tag	UNP Q9PX50
A	-24	SER	-	expression tag	UNP Q9PX50
A	-23	GLY	-	expression tag	UNP Q9PX50
A	-22	LEU	-	expression tag	UNP Q9PX50
A	-21	VAL	-	expression tag	UNP Q9PX50
A	-20	PRO	-	expression tag	UNP Q9PX50
A	-19	ARG	-	expression tag	UNP Q9PX50
A	-18	GLY	-	expression tag	UNP Q9PX50
A	-17	SER	-	expression tag	UNP Q9PX50
A	-16	HIS	-	expression tag	UNP Q9PX50
A	-15	MET	-	expression tag	UNP Q9PX50
A	-14	ALA	-	expression tag	UNP Q9PX50
A	-13	SER	-	expression tag	UNP Q9PX50
A	-12	MET	-	expression tag	UNP Q9PX50
A	-11	THR	-	expression tag	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q9PX50
A	-9	GLY	-	expression tag	UNP Q9PX50
A	-8	GLN	-	expression tag	UNP Q9PX50
A	-7	GLN	-	expression tag	UNP Q9PX50
A	-6	MET	-	expression tag	UNP Q9PX50
A	-5	GLY	-	expression tag	UNP Q9PX50
A	-4	ARG	-	expression tag	UNP Q9PX50
A	-3	GLY	-	expression tag	UNP Q9PX50
A	-2	SER	-	expression tag	UNP Q9PX50
A	-1	GLU	-	expression tag	UNP Q9PX50
A	0	PHE	-	expression tag	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	GLY	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	ILE	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	VAL	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	PRO	deletion	UNP Q9PX50
A	?	-	THR	deletion	UNP Q9PX50
A	?	-	PHE	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	VAL	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	ARG	deletion	UNP Q9PX50
A	?	-	ASN	deletion	UNP Q9PX50
A	?	-	LEU	deletion	UNP Q9PX50
A	?	-	PRO	deletion	UNP Q9PX50
A	?	-	PHE	deletion	UNP Q9PX50
A	?	-	GLU	deletion	UNP Q9PX50
A	?	-	ARG	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	THR	deletion	UNP Q9PX50
A	?	-	ILE	deletion	UNP Q9PX50
A	?	-	MET	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
B	-35	MET	-	initiating methionine	UNP Q9PX50
B	-34	GLY	-	expression tag	UNP Q9PX50
B	-33	SER	-	expression tag	UNP Q9PX50
B	-32	SER	-	expression tag	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	HIS	-	expression tag	UNP Q9PX50
B	-30	HIS	-	expression tag	UNP Q9PX50
B	-29	HIS	-	expression tag	UNP Q9PX50
B	-28	HIS	-	expression tag	UNP Q9PX50
B	-27	HIS	-	expression tag	UNP Q9PX50
B	-26	HIS	-	expression tag	UNP Q9PX50
B	-25	SER	-	expression tag	UNP Q9PX50
B	-24	SER	-	expression tag	UNP Q9PX50
B	-23	GLY	-	expression tag	UNP Q9PX50
B	-22	LEU	-	expression tag	UNP Q9PX50
B	-21	VAL	-	expression tag	UNP Q9PX50
B	-20	PRO	-	expression tag	UNP Q9PX50
B	-19	ARG	-	expression tag	UNP Q9PX50
B	-18	GLY	-	expression tag	UNP Q9PX50
B	-17	SER	-	expression tag	UNP Q9PX50
B	-16	HIS	-	expression tag	UNP Q9PX50
B	-15	MET	-	expression tag	UNP Q9PX50
B	-14	ALA	-	expression tag	UNP Q9PX50
B	-13	SER	-	expression tag	UNP Q9PX50
B	-12	MET	-	expression tag	UNP Q9PX50
B	-11	THR	-	expression tag	UNP Q9PX50
B	-10	GLY	-	expression tag	UNP Q9PX50
B	-9	GLY	-	expression tag	UNP Q9PX50
B	-8	GLN	-	expression tag	UNP Q9PX50
B	-7	GLN	-	expression tag	UNP Q9PX50
B	-6	MET	-	expression tag	UNP Q9PX50
B	-5	GLY	-	expression tag	UNP Q9PX50
B	-4	ARG	-	expression tag	UNP Q9PX50
B	-3	GLY	-	expression tag	UNP Q9PX50
B	-2	SER	-	expression tag	UNP Q9PX50
B	-1	GLU	-	expression tag	UNP Q9PX50
B	0	PHE	-	expression tag	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	GLY	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	ILE	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	VAL	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	PRO	deletion	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q9PX50
B	?	-	PHE	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	VAL	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	ARG	deletion	UNP Q9PX50
B	?	-	ASN	deletion	UNP Q9PX50
B	?	-	LEU	deletion	UNP Q9PX50
B	?	-	PRO	deletion	UNP Q9PX50
B	?	-	PHE	deletion	UNP Q9PX50
B	?	-	GLU	deletion	UNP Q9PX50
B	?	-	ARG	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	THR	deletion	UNP Q9PX50
B	?	-	ILE	deletion	UNP Q9PX50
B	?	-	MET	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50

- Molecule 2 is a DNA chain called RNA (5'-R(P*(OMU)P*(OMU)P*(OMU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	P	0	0	0
			63	30	6	24	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	30	Total	O	0	0
			30	30		

- Molecule 2: RNA (5'-R(P*(OMU)P*(OMU)P*(OMU))-3')

Chain C:  38% 62%

U1	U2	U3	OMU	OMU	OMU	OMU	OMU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.81Å 60.12Å 81.37Å 107.31° 106.68° 96.11°	Depositor
Resolution (Å)	36.61 – 3.00 36.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.1 (36.61-3.00) 86.2 (36.59-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.289 , 0.332 0.292 , 0.332	Depositor DCC
R_{free} test set	803 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , -0.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	6421	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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: OMU

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	0.62	0/3149	0.75	0/4225
1	B	0.64	0/3252	0.75	0/4366
All	All	0.63	0/6401	0.75	0/8591

There are no bond length outliers.

There are no bond angle outliers.

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	3104	0	3096	51	0
1	B	3205	0	3180	79	0
2	C	63	0	36	9	0
3	A	19	0	0	2	0
3	B	30	0	0	2	0
All	All	6421	0	6312	133	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 10.

All (133) 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)
2:C:3:OMU:O4'	2:C:3:OMU:C1'	1.64	1.29
2:C:2:OMU:O4'	2:C:2:OMU:C1'	1.65	1.23
2:C:1:OMU:O4'	2:C:1:OMU:C1'	1.65	1.19
1:B:21:ASN:HB2	1:B:24:GLU:HB2	1.44	0.96
1:B:216:ARG:HH12	1:B:244:GLU:HA	1.32	0.94
1:B:374:MET:SD	3:B:520:HOH:O	2.36	0.82
1:A:244:GLU:O	1:A:244:GLU:OE1	2.01	0.79
1:B:168:GLN:HG2	1:B:183:ILE:O	1.84	0.78
1:A:244:GLU:O	1:A:244:GLU:CD	2.23	0.76
1:B:21:ASN:CB	1:B:24:GLU:HB2	2.16	0.76
1:A:216:ARG:NH1	1:A:220:GLU:OE1	2.20	0.75
1:A:239:MET:HA	1:A:242:VAL:HG12	1.71	0.72
1:B:217:ILE:CD1	1:B:220:GLU:OE2	2.40	0.70
1:B:21:ASN:OD1	1:B:24:GLU:CG	2.40	0.69
1:B:216:ARG:NH1	1:B:244:GLU:HA	2.04	0.69
1:B:47:LEU:O	1:B:98:ARG:NH2	2.23	0.68
1:B:200:GLY:HA3	1:B:206:PHE:CE1	2.28	0.67
1:B:21:ASN:CG	1:B:24:GLU:HG2	2.16	0.67
1:A:75:ARG:HD3	1:A:174:ARG:HB2	1.77	0.66
1:A:189:MET:HB2	1:A:226:LEU:HD13	1.80	0.65
1:B:65:ARG:HB3	2:C:1:OMU:HM22	1.79	0.65
1:B:110:LEU:HD21	2:C:2:OMU:C2	2.27	0.65
1:B:217:ILE:HD13	1:B:220:GLU:OE2	2.00	0.62
1:A:172:LEU:HD11	1:A:183:ILE:HD11	1.83	0.61
1:B:193:LEU:HD21	1:B:222:MET:HG3	1.83	0.60
1:B:110:LEU:HD21	2:C:2:OMU:N1	2.16	0.60
1:A:232:THR:O	1:A:236:LYS:HG3	2.01	0.59
1:B:21:ASN:OD1	1:B:24:GLU:HG3	2.02	0.58
1:B:197:ILE:HB	1:B:253:ILE:HD11	1.85	0.57
1:B:168:GLN:CG	1:B:183:ILE:O	2.52	0.57
1:B:172:LEU:HD11	1:B:183:ILE:HD11	1.84	0.57
1:A:143:LEU:HD21	1:A:363:VAL:HG21	1.87	0.56
1:B:138:ILE:HG23	1:B:183:ILE:HD13	1.88	0.56
1:B:21:ASN:OD1	1:B:24:GLU:HG2	2.06	0.55
1:B:69:SER:OG	2:C:1:OMU:H2'	2.06	0.55
1:B:386:TRP:HZ3	1:B:388:ILE:HG23	1.70	0.55
1:B:440:MET:O	1:B:444:ILE:HD12	2.06	0.55
1:A:150:ARG:O	1:A:154:LEU:HD23	2.06	0.55
1:A:252:GLU:N	1:A:252:GLU:OE2	2.40	0.54
1:A:106:ARG:HB2	1:A:371:VAL:HG21	1.88	0.54
1:B:224:ASN:HA	1:B:227:LYS:HB3	1.90	0.53
1:B:190:VAL:HG13	1:B:256:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:HB3	1:A:55:ARG:HH12	1.73	0.52
1:B:45:THR:O	1:B:48:LYS:HD2	2.10	0.52
1:B:186:VAL:HG23	1:B:226:LEU:HD11	1.92	0.52
1:B:190:VAL:O	1:B:194:ILE:HG13	2.09	0.52
1:B:21:ASN:CG	1:B:24:GLU:CG	2.77	0.52
1:B:171:THR:HG22	1:B:171:THR:O	2.10	0.51
1:A:276:LEU:HD12	1:A:306:LEU:HD23	1.91	0.51
1:B:58:GLN:O	1:B:61:ILE:HG22	2.10	0.51
1:B:276:LEU:CD1	1:B:333:CYS:HB3	2.41	0.51
1:A:168:GLN:HG2	1:A:183:ILE:O	2.10	0.50
1:B:44:CYS:HA	1:B:49:LEU:HD12	1.93	0.50
1:A:26:ARG:HG2	1:A:296:TYR:N	2.26	0.50
1:A:242:VAL:HG23	1:A:252:GLU:CG	2.41	0.50
1:B:61:ILE:O	1:B:65:ARG:HG2	2.11	0.49
1:B:38:ARG:NH1	1:B:123:ALA:O	2.45	0.49
1:A:51:ASP:HB3	1:A:55:ARG:NH1	2.27	0.49
1:A:263:ALA:HA	1:A:266:LEU:O	2.12	0.49
1:A:355:ARG:HA	1:A:358:LEU:HD12	1.95	0.49
1:A:495:GLU:HG3	3:A:501:HOH:O	2.12	0.49
1:A:26:ARG:HG2	1:A:296:TYR:H	1.77	0.49
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.95	0.48
1:B:242:VAL:HA	1:B:252:GLU:OE1	2.13	0.48
1:A:152:ARG:HD3	1:A:495:GLU:OE2	2.14	0.48
1:A:230:PHE:HB3	1:A:235:GLN:HG3	1.96	0.48
1:B:327:GLN:HE21	1:B:331:MET:HE1	1.77	0.48
1:B:106:ARG:HB2	1:B:371:VAL:HG21	1.95	0.47
1:B:263:ALA:HA	1:B:266:LEU:O	2.13	0.47
1:A:361:ARG:HE	1:A:361:ARG:HB3	1.42	0.47
1:B:317:ARG:HB2	1:B:320:GLU:CD	2.34	0.47
1:B:227:LYS:HE3	1:B:236:LYS:HB3	1.96	0.47
1:A:217:ILE:HG22	1:A:221:ARG:NH2	2.30	0.47
1:A:317:ARG:HB2	1:A:320:GLU:CD	2.34	0.46
1:B:348:ARG:HD3	1:B:350:THR:HG23	1.98	0.46
1:B:346:PHE:CZ	1:B:477:PRO:HA	2.50	0.46
1:A:25:ILE:HD12	1:A:25:ILE:HA	1.68	0.46
1:A:248:PRO:HA	1:A:252:GLU:OE1	2.14	0.46
1:B:170:SER:HA	1:B:188:THR:HG23	1.96	0.46
1:B:200:GLY:HA3	1:B:206:PHE:CZ	2.50	0.46
1:B:217:ILE:HD12	1:B:220:GLU:OE2	2.14	0.46
1:A:186:VAL:HG13	1:A:226:LEU:HD11	1.98	0.46
1:B:194:ILE:HG23	1:B:253:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:OD1	1:B:243:ARG:NH2	2.49	0.45
1:B:171:THR:HG23	1:B:496:TYR:CZ	2.51	0.45
1:B:276:LEU:HB2	1:B:281:TYR:CZ	2.52	0.45
1:A:323:ALA:HB2	1:B:152:ARG:NH1	2.32	0.45
1:A:143:LEU:HD21	1:A:363:VAL:CG2	2.47	0.45
1:B:23:THR:O	1:B:26:ARG:N	2.50	0.45
1:B:386:TRP:CZ3	1:B:388:ILE:HG23	2.50	0.45
1:A:115:GLU:OE2	1:A:118:ARG:NH2	2.48	0.44
2:C:2:OMU:HM23	2:C:2:OMU:H1'	1.77	0.44
1:A:266:LEU:HD11	1:A:447:MET:HG3	2.00	0.44
1:A:33:VAL:HG13	1:A:281:TYR:CD1	2.52	0.44
1:B:73:GLU:H	1:B:73:GLU:HG3	1.57	0.44
1:B:380:GLU:OE1	1:B:382:ARG:N	2.49	0.44
1:A:341:LEU:HD22	1:A:352:VAL:HG12	2.00	0.44
1:B:98:ARG:HD2	1:B:107:GLU:OE1	2.18	0.44
1:A:276:LEU:HD22	1:A:307:LEU:HD21	2.00	0.43
1:A:444:ILE:O	1:A:448:MET:HG3	2.17	0.43
1:A:137:MET:HE1	1:A:176:SER:HB2	2.00	0.43
1:B:346:PHE:HZ	1:B:475:ILE:HG22	1.83	0.43
1:A:444:ILE:HG22	1:A:448:MET:HE2	2.00	0.43
1:A:99:ARG:HD2	1:A:99:ARG:HA	1.83	0.43
1:B:441:ARG:O	1:B:445:ILE:HD12	2.19	0.43
1:A:261:ARG:HG3	3:A:513:HOH:O	2.18	0.43
1:B:216:ARG:CG	1:B:216:ARG:HH21	2.31	0.42
1:A:72:ASP:OD1	1:A:75:ARG:N	2.53	0.42
1:B:217:ILE:HA	1:B:220:GLU:HG2	2.01	0.42
1:B:134:THR:O	1:B:138:ILE:HG13	2.19	0.42
1:B:99:ARG:HA	1:B:99:ARG:HD2	1.88	0.42
1:B:137:MET:SD	1:B:176:SER:OG	2.62	0.42
1:B:72:ASP:O	1:B:76:ASN:N	2.52	0.42
1:A:56:LEU:HD11	1:A:315:LEU:HG	2.02	0.41
1:B:300:GLY:HA2	1:B:388:ILE:HG22	2.01	0.41
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.86	0.41
1:B:444:ILE:O	1:B:448:MET:HG3	2.20	0.41
1:A:99:ARG:O	1:A:100:ARG:NH1	2.43	0.41
1:A:331:MET:HE3	1:A:331:MET:HB3	1.77	0.41
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.92	0.41
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.85	0.41
1:B:341:LEU:HD22	1:B:352:VAL:HG12	2.03	0.41
1:A:66:MET:SD	1:A:109:ILE:HD11	2.61	0.41
1:B:110:LEU:HD21	2:C:2:OMU:C6	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:NH2	1:B:216:ARG:HG3	2.35	0.41
1:B:387:ALA:HA	1:B:462:GLY:O	2.20	0.41
1:A:276:LEU:HB2	1:A:281:TYR:CZ	2.56	0.40
1:B:150:ARG:HD2	3:B:504:HOH:O	2.20	0.40
1:A:144:ASN:HB3	1:A:171:THR:HG21	2.03	0.40
1:B:168:GLN:HE21	1:B:183:ILE:HB	1.87	0.40
1:B:138:ILE:HG23	1:B:183:ILE:CD1	2.50	0.40
1:B:42:GLN:OE1	1:B:119:ILE:HG23	2.22	0.40
1:B:308:GLN:HA	1:B:382:ARG:HG2	2.02	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	381/505 (75%)	368 (97%)	12 (3%)	1 (0%)	41	76
1	B	397/505 (79%)	384 (97%)	13 (3%)	0	100	100
All	All	778/1010 (77%)	752 (97%)	25 (3%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	GLU

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	329/420 (78%)	318 (97%)	11 (3%)	38	73
1	B	337/420 (80%)	329 (98%)	8 (2%)	49	79
All	All	666/840 (79%)	647 (97%)	19 (3%)	42	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	73	GLU
1	A	76	ASN
1	A	115	GLU
1	A	239	MET
1	A	361	ARG
1	A	367	SER
1	A	441	ARG
1	A	446	ARG
1	A	450	SER
1	A	494	GLU
1	B	21	ASN
1	B	73	GLU
1	B	74	ARG
1	B	168	GLN
1	B	216	ARG
1	B	243	ARG
1	B	350	THR
1	B	440	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	327	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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
2	OMU	C	1	2	19,22,23	4.75	12 (63%)	25,31,34	2.07	8 (32%)
2	OMU	C	2	2	19,22,23	4.37	11 (57%)	25,31,34	2.01	6 (24%)
2	OMU	C	3	2	19,22,23	4.44	11 (57%)	25,31,34	1.89	7 (28%)

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
2	OMU	C	1	2	-	3/9/27/28	0/2/2/2
2	OMU	C	2	2	-	1/9/27/28	0/2/2/2
2	OMU	C	3	2	-	1/9/27/28	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	OMU	O4'-C1'	10.09	1.65	1.42
2	C	2	OMU	O4'-C1'	9.95	1.65	1.42
2	C	3	OMU	O4'-C1'	9.86	1.64	1.42
2	C	1	OMU	C2-N3	8.24	1.52	1.38
2	C	1	OMU	C2-N1	8.03	1.51	1.38
2	C	3	OMU	C2-N3	7.71	1.51	1.38
2	C	2	OMU	C2-N1	7.35	1.50	1.38
2	C	3	OMU	C2-N1	6.89	1.49	1.38
2	C	2	OMU	C2-N3	6.79	1.49	1.38
2	C	1	OMU	C2'-C1'	-6.59	1.36	1.53
2	C	1	OMU	C6-C5	6.52	1.50	1.35
2	C	1	OMU	O4'-C4'	-6.07	1.31	1.45
2	C	2	OMU	C2'-C1'	-6.06	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	OMU	C2'-C1'	-6.01	1.38	1.53
2	C	3	OMU	O4'-C4'	-5.82	1.32	1.45
2	C	2	OMU	C6-C5	5.61	1.48	1.35
2	C	3	OMU	C6-C5	5.56	1.48	1.35
2	C	2	OMU	O4'-C4'	-5.28	1.33	1.45
2	C	1	OMU	C4-N3	5.06	1.47	1.38
2	C	2	OMU	C4-N3	4.40	1.46	1.38
2	C	3	OMU	C4-N3	4.29	1.46	1.38
2	C	2	OMU	O3'-C3'	-3.67	1.33	1.43
2	C	3	OMU	C6-N1	3.35	1.46	1.38
2	C	2	OMU	C6-N1	3.29	1.45	1.38
2	C	1	OMU	O3'-C3'	-3.13	1.35	1.43
2	C	3	OMU	C3'-C4'	3.12	1.60	1.53
2	C	1	OMU	C6-N1	3.06	1.45	1.38
2	C	3	OMU	O2'-C2'	3.01	1.50	1.42
2	C	3	OMU	O3'-C3'	-2.95	1.35	1.43
2	C	1	OMU	C3'-C4'	2.72	1.59	1.53
2	C	2	OMU	O2'-C2'	2.47	1.48	1.42
2	C	1	OMU	O2'-C2'	2.43	1.48	1.42
2	C	1	OMU	C5-C4	2.35	1.48	1.43
2	C	2	OMU	C3'-C4'	2.23	1.58	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	OMU	C4-N3-C2	-5.24	120.10	126.61
2	C	2	OMU	C4-N3-C2	-4.92	120.50	126.61
2	C	3	OMU	C4-N3-C2	-4.52	121.00	126.61
2	C	1	OMU	N3-C2-N1	4.33	120.53	114.89
2	C	2	OMU	C5-C4-N3	3.99	120.39	114.80
2	C	2	OMU	O4-C4-C5	-3.68	118.81	125.16
2	C	3	OMU	C5-C4-N3	3.33	119.47	114.80
2	C	1	OMU	O4-C4-C5	-3.25	119.56	125.16
2	C	2	OMU	N3-C2-N1	3.25	119.12	114.89
2	C	1	OMU	O2-C2-N1	-3.16	118.69	122.80
2	C	3	OMU	C3'-C2'-C1'	3.01	108.58	102.81
2	C	3	OMU	O4-C4-C5	-2.98	120.03	125.16
2	C	3	OMU	N3-C2-N1	2.93	118.70	114.89
2	C	3	OMU	O2-C2-N1	-2.77	119.19	122.80
2	C	1	OMU	C5-C4-N3	2.74	118.64	114.80
2	C	1	OMU	C2'-C1'-N1	2.62	119.21	114.24
2	C	3	OMU	O2'-C2'-C1'	2.60	113.92	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	OMU	O2'-C2'-C1'	2.44	113.62	108.99
2	C	1	OMU	C6-N1-C2	-2.34	118.14	121.00
2	C	2	OMU	O4'-C1'-N1	2.01	112.92	108.36
2	C	1	OMU	O3'-C3'-C2'	2.00	116.79	111.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	OMU	C1'-C2'-O2'-CM2
2	C	2	OMU	C1'-C2'-O2'-CM2
2	C	1	OMU	C3'-C4'-C5'-O5'
2	C	1	OMU	O4'-C4'-C5'-O5'
2	C	3	OMU	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	OMU	3	0
2	C	2	OMU	5	0
2	C	3	OMU	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, 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	393/505 (77%)	-0.33	2 (0%) 91 75	14, 31, 68, 92	0
1	B	409/505 (80%)	-0.44	0 100 100	10, 28, 64, 90	0
2	C	0/8	-	-	-	-
All	All	802/1018 (78%)	-0.39	2 (0%) 95 87	10, 30, 66, 92	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ARG	3.6
1	A	175	ARG	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
2	OMU	C	1	21/22	0.88	0.23	39,48,60,64	0
2	OMU	C	3	21/22	0.90	0.19	43,50,58,62	0
2	OMU	C	2	21/22	0.95	0.14	33,42,45,47	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.