Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 05:13 PM JST

PDB ID	:	7DXP
Title	:	Influenza H5N1 nucleoprotein in complex with nucleotides
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Deposited on	:	2021-01-19
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

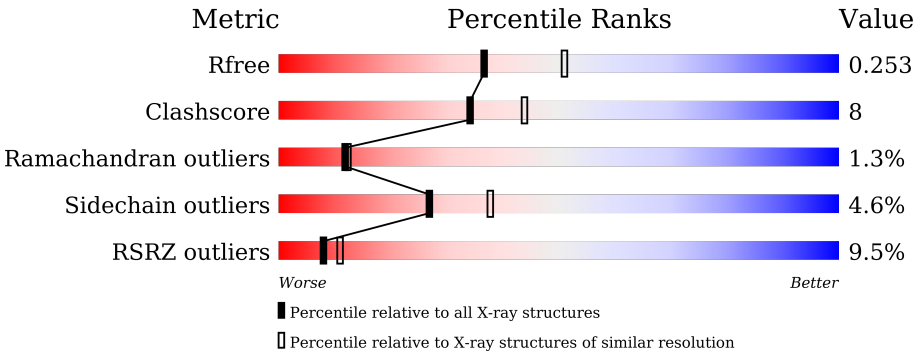
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	507	8% 67% 10% . 21%
1	B	507	8% 68% 13% . 18%
2	C	9	11% 33% 56%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6727 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.

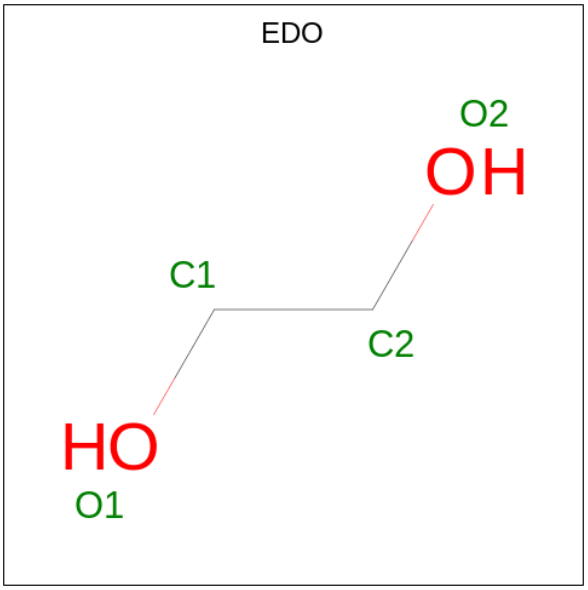
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	1	0
			3161	1966	585	584	26			
1	B	418	Total	C	N	O	S	0	3	0
			3337	2066	632	613	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			66	30	6	26	4			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

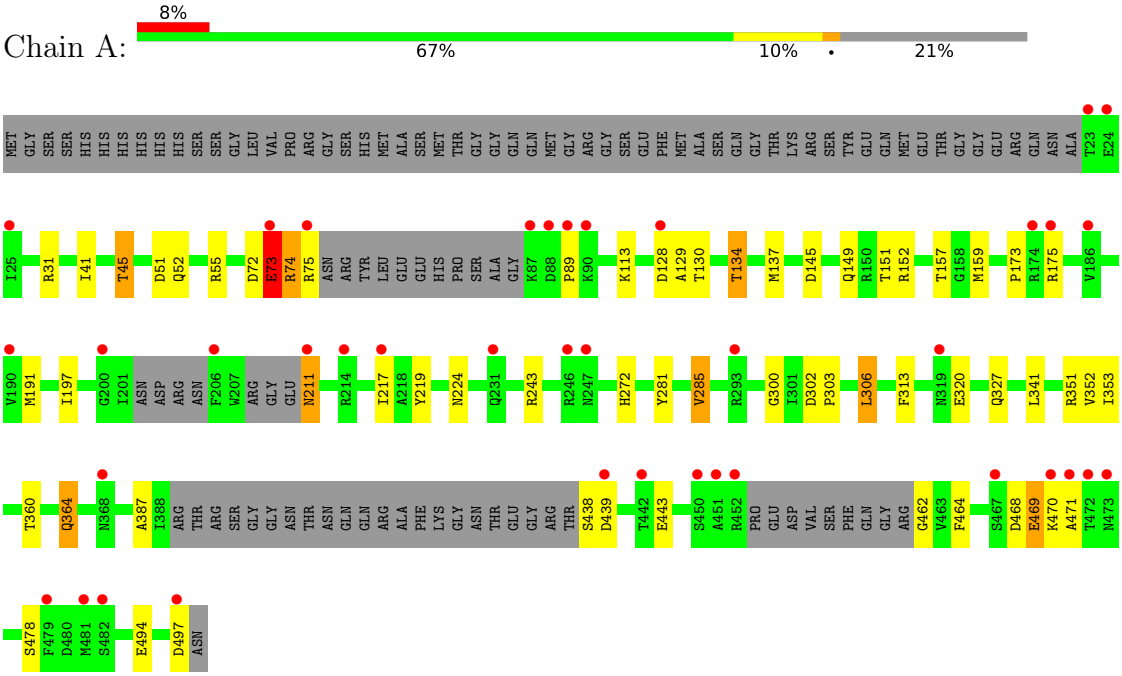
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	B	92	Total O 92 92	0	0

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.

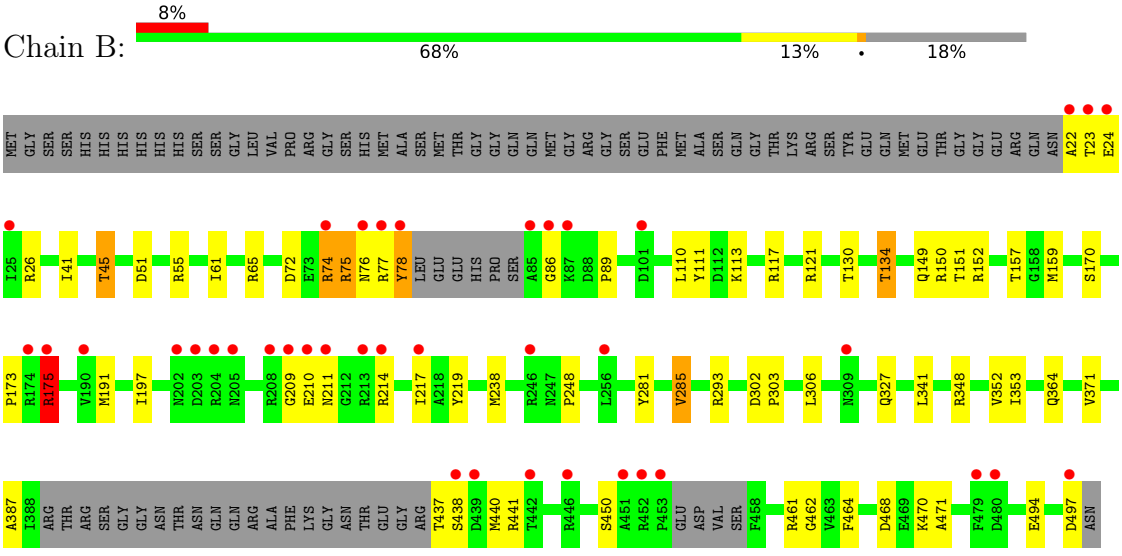
• Molecule 1: Nucleoprotein

Chain A:



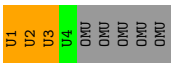
• Molecule 1: Nucleoprotein

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.01Å 60.63Å 82.71Å 106.70° 109.01° 96.62°	Depositor
Resolution (Å)	24.50 – 2.30 24.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.3 (24.50-2.30) 90.4 (24.46-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.248 0.202 , 0.253	Depositor DCC
R_{free} test set	1866 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6727	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO

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	0.76	1/3213 (0.0%)	0.90	1/4312 (0.0%)
1	B	0.78	0/3392	0.94	3/4551 (0.1%)
All	All	0.77	1/6605 (0.0%)	0.92	4/8863 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLU	CD-OE1	5.09	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	348	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	351	ARG	CG-CD-NE	-5.31	100.65	111.80
1	B	117	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	3161	0	3146	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3337	0	3318	62	0
2	C	66	0	36	6	0
3	A	4	0	6	3	0
3	B	4	0	6	1	0
4	A	63	0	0	2	0
4	B	92	0	0	2	0
All	All	6727	0	6512	110	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 8.

All (110) 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:2:OMU:O4'	2:C:2:OMU:C1'	1.63	1.30
2:C:1:OMU:O4'	2:C:1:OMU:C1'	1.66	1.24
2:C:3:OMU:O4'	2:C:3:OMU:C1'	1.67	1.23
1:B:121[B]:ARG:HH11	1:B:121[B]:ARG:HG2	1.00	1.09
1:B:121[B]:ARG:HH11	1:B:121[B]:ARG:CG	1.75	0.95
1:A:74:ARG:HD2	1:A:173:PRO:HG2	1.56	0.88
1:B:175[A]:ARG:HH21	1:B:175[A]:ARG:CG	1.86	0.87
1:B:121[B]:ARG:HG2	1:B:121[B]:ARG:NH1	1.84	0.85
1:B:175[A]:ARG:HH21	1:B:175[A]:ARG:HG2	1.39	0.85
1:B:159:MET:SD	4:B:684:HOH:O	2.36	0.83
1:B:157:THR:CG2	1:B:159:MET:HE2	2.18	0.73
1:B:157:THR:HG21	1:B:159:MET:HE2	1.70	0.72
1:A:149:GLN:NE2	1:A:151:THR:OG1	2.23	0.72
1:A:152:ARG:NH2	1:A:497:ASP:OD2	2.24	0.69
1:A:159:MET:HE1	1:A:191:MET:HB2	1.73	0.69
1:A:211:ASN:HD22	1:A:211:ASN:C	1.95	0.69
1:B:175[A]:ARG:HB3	1:B:175[A]:ARG:NH2	2.06	0.69
1:B:175[A]:ARG:HH21	1:B:175[A]:ARG:CB	2.04	0.69
1:B:152:ARG:NH2	1:B:497:ASP:OD2	2.25	0.68
3:A:501:EDO:H21	4:A:649:HOH:O	1.95	0.67
1:B:149:GLN:NE2	1:B:151:THR:OG1	2.28	0.67
1:A:130:THR:O	1:A:134:THR:HG23	1.95	0.66
1:B:327:GLN:HE22	1:B:353:ILE:H	1.44	0.66
1:A:157:THR:CG2	1:A:159:MET:HE2	2.27	0.65
1:A:157:THR:HG21	1:A:159:MET:HE2	1.78	0.65
1:B:159:MET:HE1	1:B:191:MET:HB2	1.79	0.65
1:A:128:ASP:O	1:A:130:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:MET:HE1	1:B:191:MET:CB	2.28	0.64
1:B:175[A]:ARG:NH2	1:B:175[A]:ARG:CB	2.61	0.64
1:A:159:MET:HE1	1:A:191:MET:CB	2.27	0.64
1:A:145:ASP:HA	3:A:501:EDO:H21	1.81	0.63
1:A:327:GLN:HE22	1:A:353:ILE:H	1.47	0.62
1:B:121[B]:ARG:CG	1:B:121[B]:ARG:NH1	2.44	0.61
1:B:468:ASP:OD1	1:B:470:LYS:O	2.19	0.60
1:B:175[A]:ARG:HH21	1:B:175[A]:ARG:H	1.50	0.60
1:B:464:PHE:CZ	1:B:471:ALA:HB1	2.37	0.59
1:A:89:PRO:O	1:A:113:LYS:HE2	2.01	0.58
1:A:468:ASP:OD1	1:A:470:LYS:O	2.20	0.58
1:A:464:PHE:CZ	1:A:471:ALA:HB1	2.39	0.58
1:B:89:PRO:O	1:B:113:LYS:HE2	2.04	0.57
1:A:41:ILE:HD12	1:A:285:VAL:HG22	1.87	0.56
1:B:327:GLN:NE2	1:B:353:ILE:H	2.04	0.55
1:B:76:ASN:O	1:B:78:TYR:N	2.38	0.55
1:A:72:ASP:O	1:A:74:ARG:N	2.38	0.55
1:A:327:GLN:NE2	1:A:353:ILE:H	2.04	0.55
1:B:130:THR:O	1:B:134:THR:HG23	2.07	0.54
1:B:41:ILE:CD1	1:B:285:VAL:HG22	2.37	0.54
1:B:65:ARG:HD3	3:B:501:EDO:O1	2.07	0.54
1:B:175[A]:ARG:NH2	1:B:175[A]:ARG:H	2.05	0.54
1:A:74:ARG:HD3	1:A:137:MET:HE2	1.91	0.53
1:A:52:GLN:NE2	1:A:313:PHE:HE2	2.07	0.53
1:B:175[A]:ARG:HG2	1:B:175[A]:ARG:NH2	2.17	0.52
1:A:41:ILE:CD1	1:A:285:VAL:HG22	2.39	0.52
1:A:327:GLN:HE22	1:A:353:ILE:HG12	1.73	0.52
1:B:302:ASP:HB2	1:B:303:PRO:HD3	1.91	0.52
1:B:150:ARG:HD3	1:B:170:SER:OG	2.10	0.52
1:B:197:ILE:HD11	1:B:219:TYR:HE1	1.75	0.51
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.93	0.51
1:B:437:THR:HA	1:B:440:MET:HE1	1.92	0.51
1:B:152:ARG:NH2	4:B:604:HOH:O	2.44	0.51
1:A:74:ARG:HH21	1:A:137:MET:HG3	1.76	0.51
1:B:61:ILE:HG21	1:B:364:GLN:NE2	2.26	0.50
1:B:41:ILE:O	1:B:45:THR:HG23	2.12	0.50
1:B:26:ARG:NH2	1:B:302:ASP:OD2	2.45	0.49
1:B:209:GLY:O	1:B:211:ASN:N	2.44	0.49
1:A:52:GLN:NE2	1:A:313:PHE:CE2	2.81	0.49
1:B:175[A]:ARG:CG	1:B:175[A]:ARG:NH2	2.56	0.49
1:B:41:ILE:HD12	1:B:285:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:MET:HE1	1:B:441:ARG:HG3	1.95	0.48
1:A:197:ILE:HD11	1:A:219:TYR:HE1	1.79	0.48
1:B:22:ALA:C	1:B:24:GLU:H	2.17	0.48
1:B:327:GLN:HE22	1:B:353:ILE:HG12	1.79	0.47
1:A:281:TYR:O	1:A:285:VAL:HG13	2.15	0.47
1:A:469:GLU:HG3	1:A:470:LYS:H	1.80	0.46
1:B:173:PRO:HB2	1:B:175[A]:ARG:HG2	1.97	0.46
1:B:437:THR:HA	1:B:440:MET:CE	2.45	0.46
1:A:41:ILE:O	1:A:45:THR:HG23	2.14	0.46
2:C:1:OMU:H5"	2:C:1:OMU:H6	1.97	0.46
1:A:145:ASP:HA	3:A:501:EDO:C2	2.45	0.45
1:A:364:GLN:HE21	1:A:364:GLN:HA	1.82	0.45
1:B:341:LEU:HD22	1:B:352:VAL:HG12	1.99	0.45
1:B:197:ILE:HD12	1:B:248:PRO:HB3	1.99	0.45
1:B:74:ARG:N	1:B:75:ARG:HD2	2.32	0.44
1:A:387:ALA:HA	1:A:462:GLY:O	2.17	0.44
1:B:110:LEU:HD13	2:C:2:OMU:C2	2.48	0.43
1:B:211:ASN:O	1:B:214:ARG:HB2	2.17	0.43
1:B:387:ALA:HA	1:B:462:GLY:O	2.17	0.43
1:A:300:GLY:HA3	4:A:636:HOH:O	2.17	0.43
1:B:72:ASP:O	1:B:75:ARG:CZ	2.66	0.43
1:A:51:ASP:HB3	1:A:55:ARG:HH12	1.84	0.43
1:B:281:TYR:O	1:B:285:VAL:HG13	2.19	0.43
1:A:341:LEU:HD22	1:A:352:VAL:HG12	2.01	0.42
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.82	0.42
1:A:211:ASN:C	1:A:211:ASN:ND2	2.68	0.42
1:B:159:MET:HE1	1:B:191:MET:CG	2.49	0.42
1:B:75:ARG:N	1:B:75:ARG:HE	2.17	0.42
1:B:51:ASP:HB3	1:B:55:ARG:HH12	1.84	0.42
1:B:75:ARG:NH2	1:B:113:LYS:HE3	2.34	0.42
1:A:72:ASP:C	1:A:74:ARG:H	2.21	0.41
1:B:22:ALA:C	1:B:24:GLU:N	2.73	0.41
1:B:78:TYR:C	1:B:78:TYR:CD1	2.94	0.41
1:B:78:TYR:C	1:B:78:TYR:HD1	2.24	0.41
1:A:224:ASN:OD1	1:A:243:ARG:NH1	2.54	0.41
1:B:75:ARG:CZ	1:B:113:LYS:HE3	2.51	0.41
1:A:73:GLU:O	1:A:74:ARG:HG3	2.20	0.41
1:A:149:GLN:HE21	1:A:151:THR:CG2	2.34	0.40
1:B:175[A]:ARG:HB3	1:B:175[A]:ARG:CZ	2.52	0.40
1:B:74:ARG:NH1	2:C:1:OMU:OP1	2.51	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	388/507 (76%)	376 (97%)	8 (2%)	4 (1%)	15 17
1	B	413/507 (82%)	396 (96%)	10 (2%)	7 (2%)	9 8
All	All	801/1014 (79%)	772 (96%)	18 (2%)	11 (1%)	12 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ALA
1	B	23	THR
1	B	77	ARG
1	B	210	GLU
1	B	461	ARG
1	A	73	GLU
1	A	74	ARG
1	A	175	ARG
1	B	86	GLY
1	B	175[A]	ARG
1	B	175[B]	ARG

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	335/422 (79%)	318 (95%)	17 (5%)	24 33
1	B	350/422 (83%)	335 (96%)	15 (4%)	29 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	685/844 (81%)	653 (95%)	32 (5%)	27 37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	45	THR
1	A	73	GLU
1	A	75	ARG
1	A	134	THR
1	A	211	ASN
1	A	217	ILE
1	A	285	VAL
1	A	306	LEU
1	A	360	THR
1	A	364	GLN
1	A	438	SER
1	A	439	ASP
1	A	443	GLU
1	A	469	GLU
1	A	478	SER
1	A	494	GLU
1	B	45	THR
1	B	74	ARG
1	B	75	ARG
1	B	78	TYR
1	B	111	TYR
1	B	134	THR
1	B	175[A]	ARG
1	B	175[B]	ARG
1	B	217	ILE
1	B	285	VAL
1	B	306	LEU
1	B	371	VAL
1	B	438	SER
1	B	450	SER
1	B	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	149	GLN
1	A	168	GLN
1	A	211	ASN
1	A	327	GLN
1	A	364	GLN
1	B	52	GLN
1	B	149	GLN
1	B	327	GLN
1	B	364	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	4	2	0,2,23	-	-	0,1,34	-	-
2	OMU	C	3	2	19,22,23	4.52	13 (68%)	26,31,34	2.22	8 (30%)
2	OMU	C	2	2	19,22,23	4.41	11 (57%)	26,31,34	2.03	8 (30%)
2	OMU	C	1	2	19,22,23	4.77	12 (63%)	26,31,34	2.54	10 (38%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	C	1	2	-	4/9/27/28	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	OMU	O4'-C1'	10.95	1.67	1.42
2	C	1	OMU	O4'-C1'	10.11	1.66	1.42
2	C	2	OMU	O4'-C1'	9.24	1.63	1.42
2	C	1	OMU	C2-N1	7.57	1.50	1.38
2	C	3	OMU	C2-N3	7.36	1.51	1.38
2	C	1	OMU	C2'-C1'	-7.32	1.34	1.53
2	C	1	OMU	C2-N3	7.19	1.50	1.38
2	C	2	OMU	C2-N3	7.18	1.50	1.38
2	C	2	OMU	C2-N1	7.01	1.49	1.38
2	C	1	OMU	O4'-C4'	-6.82	1.29	1.45
2	C	2	OMU	C2'-C1'	-6.70	1.35	1.53
2	C	3	OMU	C2'-C1'	-6.58	1.36	1.53
2	C	3	OMU	C2-N1	6.40	1.48	1.38
2	C	2	OMU	C6-C5	6.36	1.49	1.35
2	C	1	OMU	C6-C5	6.19	1.49	1.35
2	C	3	OMU	C6-C5	6.13	1.49	1.35
2	C	2	OMU	O4'-C4'	-5.49	1.32	1.45
2	C	3	OMU	O4'-C4'	-5.48	1.32	1.45
2	C	1	OMU	O2'-C2'	4.18	1.53	1.42
2	C	1	OMU	O3'-C3'	-3.96	1.33	1.43
2	C	2	OMU	O3'-C3'	-3.89	1.33	1.43
2	C	1	OMU	C4-N3	3.82	1.45	1.38
2	C	2	OMU	C4-N3	3.53	1.44	1.38
2	C	2	OMU	O2'-C2'	3.35	1.51	1.42
2	C	3	OMU	C4-N3	3.26	1.44	1.38
2	C	2	OMU	C5-C4	3.25	1.50	1.43
2	C	1	OMU	C3'-C4'	3.20	1.61	1.53
2	C	3	OMU	O3'-C3'	-3.16	1.35	1.43
2	C	3	OMU	O2'-C2'	3.07	1.50	1.42
2	C	2	OMU	C6-N1	3.02	1.45	1.38
2	C	1	OMU	C6-N1	2.93	1.45	1.38
2	C	3	OMU	C6-N1	2.92	1.45	1.38
2	C	3	OMU	C3'-C4'	2.76	1.60	1.53
2	C	1	OMU	C5-C4	2.67	1.49	1.43
2	C	3	OMU	O2-C2	-2.49	1.18	1.23
2	C	3	OMU	C5-C4	2.49	1.49	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	OMU	C4-N3-C2	-6.65	117.80	126.58
2	C	3	OMU	N3-C2-N1	5.83	122.62	114.89
2	C	1	OMU	N3-C2-N1	5.76	122.53	114.89
2	C	3	OMU	C4-N3-C2	-5.72	119.03	126.58
2	C	2	OMU	C4-N3-C2	-4.72	120.35	126.58
2	C	1	OMU	O2-C2-N1	-4.56	116.73	122.79
2	C	2	OMU	N3-C2-N1	4.29	120.58	114.89
2	C	2	OMU	O2-C2-N1	-3.75	117.80	122.79
2	C	1	OMU	CM2-O2'-C2'	3.56	123.88	114.52
2	C	3	OMU	C6-N1-C2	-3.30	116.77	120.99
2	C	1	OMU	C5-C4-N3	3.26	119.72	114.84
2	C	1	OMU	C1'-N1-C6	3.18	127.78	120.84
2	C	3	OMU	C2'-C1'-N1	3.14	120.33	114.22
2	C	3	OMU	C5-C4-N3	2.95	119.26	114.84
2	C	2	OMU	C4'-O4'-C1'	-2.86	103.16	109.47
2	C	2	OMU	C5-C4-N3	2.78	119.00	114.84
2	C	1	OMU	C2'-C3'-C4'	2.59	107.62	101.99
2	C	1	OMU	C1'-N1-C2	-2.22	113.55	117.57
2	C	3	OMU	O2-C2-N3	-2.21	117.39	121.50
2	C	2	OMU	O4'-C1'-N1	2.15	113.27	108.36
2	C	2	OMU	C5'-C4'-C3'	-2.14	107.15	115.18
2	C	2	OMU	C1'-N1-C6	2.13	125.48	120.84
2	C	1	OMU	O2'-C2'-C1'	2.12	113.21	109.08
2	C	3	OMU	O2-C2-N1	-2.11	119.99	122.79
2	C	1	OMU	O4-C4-C5	-2.06	121.54	125.16
2	C	3	OMU	O3'-C3'-C2'	2.05	116.99	111.17

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	1	OMU	C3'-C4'-C5'-O5'
2	C	1	OMU	O4'-C4'-C5'-O5'
2	C	1	OMU	C4'-C5'-O5'-P
2	C	3	OMU	C3'-C2'-O2'-CM2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	OMU	1	0
2	C	2	OMU	2	0
2	C	1	OMU	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
3	EDO	A	501	-	3,3,3	0.76	0	2,2,2	0.90	0
3	EDO	B	501	-	3,3,3	0.57	0	2,2,2	0.66	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
3	EDO	A	501	-	-	1/1/1/1	-
3	EDO	B	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	501	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	EDO	3	0
3	B	501	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	399/507 (78%)	0.42	39 (9%)	7	10	16, 35, 72, 99	0
1	B	418/507 (82%)	0.37	39 (9%)	8	11	14, 30, 69, 97	1 (0%)
2	C	0/9	-	-			-	-
All	All	817/1023 (79%)	0.39	78 (9%)	8	11	14, 32, 71, 99	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	ALA	6.0
1	A	73	GLU	5.8
1	B	205	ASN	5.2
1	B	214	ARG	5.1
1	A	89	PRO	4.8
1	B	210	GLU	4.5
1	B	453	PRO	4.4
1	A	87	LYS	4.3
1	B	23	THR	4.3
1	B	209	GLY	4.3
1	B	22	ALA	4.2
1	A	25	ILE	4.2
1	B	74	ARG	4.1
1	A	24	GLU	4.1
1	B	203	ASP	4.0
1	A	75	ARG	3.9
1	A	246	ARG	3.9
1	A	214	ARG	3.9
1	B	202	ASN	3.8
1	B	208	ARG	3.8
1	A	450	SER	3.7
1	B	76	ASN	3.7
1	B	78	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	246	ARG	3.6
1	A	442	THR	3.6
1	A	439	ASP	3.5
1	B	204	ARG	3.3
1	A	451	ALA	3.3
1	B	442	THR	3.2
1	B	174	ARG	3.2
1	A	88	ASP	3.2
1	A	211	ASN	3.2
1	A	217	ILE	3.1
1	B	25	ILE	3.1
1	B	452	ARG	3.1
1	A	293	ARG	3.0
1	B	24	GLU	3.0
1	B	213	ARG	3.0
1	A	190	VAL	3.0
1	A	174	ARG	2.9
1	A	472	THR	2.9
1	A	452	ARG	2.9
1	A	319	ASN	2.8
1	A	479	PHE	2.8
1	B	451	ALA	2.8
1	B	175[A]	ARG	2.7
1	B	479	PHE	2.7
1	A	206	PHE	2.7
1	B	438	SER	2.6
1	A	23	THR	2.6
1	B	480	ASP	2.6
1	B	497	ASP	2.6
1	A	481	MET	2.5
1	B	86	GLY	2.5
1	A	175	ARG	2.5
1	A	473	ASN	2.4
1	B	211	ASN	2.4
1	A	231	GLN	2.4
1	A	467	SER	2.4
1	A	470	LYS	2.3
1	B	217	ILE	2.3
1	B	256	LEU	2.3
1	B	190	VAL	2.3
1	A	128	ASP	2.3
1	A	368	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	439	ASP	2.3
1	B	446	ARG	2.2
1	A	186	VAL	2.2
1	A	200	GLY	2.2
1	B	101	ASP	2.2
1	B	309	ASN	2.1
1	B	77	ARG	2.1
1	A	247	ASN	2.1
1	A	471	ALA	2.0
1	A	482	SER	2.0
1	A	90	LYS	2.0
1	A	497	ASP	2.0
1	B	87	LYS	2.0

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, 95^{th} 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	0.82	0.22	43,54,74,77	0
2	OMU	C	4	3/22	0.87	0.31	67,67,71,74	0
2	OMU	C	3	21/22	0.93	0.14	33,40,57,68	0
2	OMU	C	2	21/22	0.96	0.11	38,43,53,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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
3	EDO	A	501	4/4	0.89	0.20	33,41,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	501	4/4	0.90	0.28	34,42,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.