



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:27 am GMT

PDB ID : 4OAV
Title : Complete human RNase L in complex with 2-5A (5'-ppp heptamer), AMPPCP and RNA substrate.
Authors : Han, Y.; Donovan, J.; Rath, S.; Whitney, G.; Chitrakar, A.; Korennykh, A.
Deposited on : 2014-01-06
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

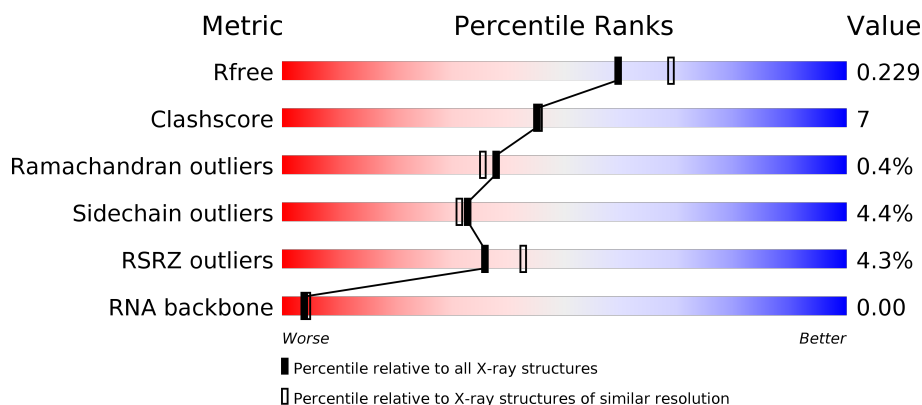
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


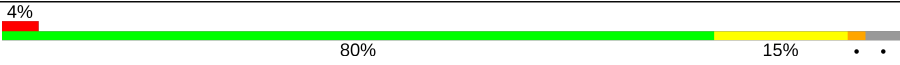
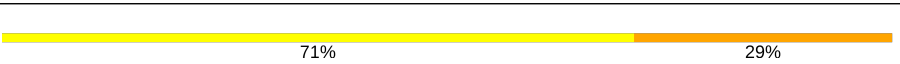
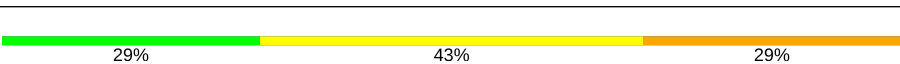
The reported resolution of this entry is 2.10 Å.

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)
RNA backbone	2435	1063 (2.70-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	699	
1	D	699	
2	A	7	
2	C	7	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11963 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 PROTEIN (RNase L).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	673	Total	C	N	O	S	0	0	0
			5372	3397	943	1010	22			
1	D	674	Total	C	N	O	S	0	0	0
			5379	3400	945	1012	22			

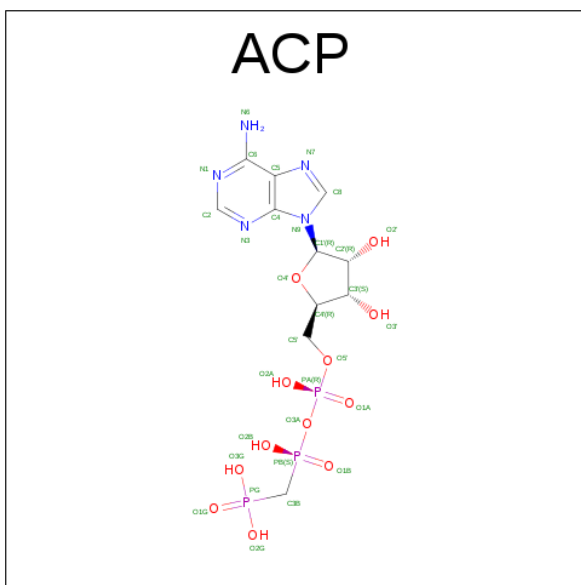
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	672	ASN	HIS	ENGINEERED MUTATION	UNP Q05823
D	672	ASN	HIS	ENGINEERED MUTATION	UNP Q05823

- Molecule 2 is a RNA chain called RNA (5'-R(P*(PO4)P*(PO4)P*AP*AP*AP*AP*(PO4))-2').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	7	Total	C	N	O	P	0	0	0
			101	40	20	34	7			
2	C	7	Total	C	N	O	P	0	0	0
			101	40	20	34	7			

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

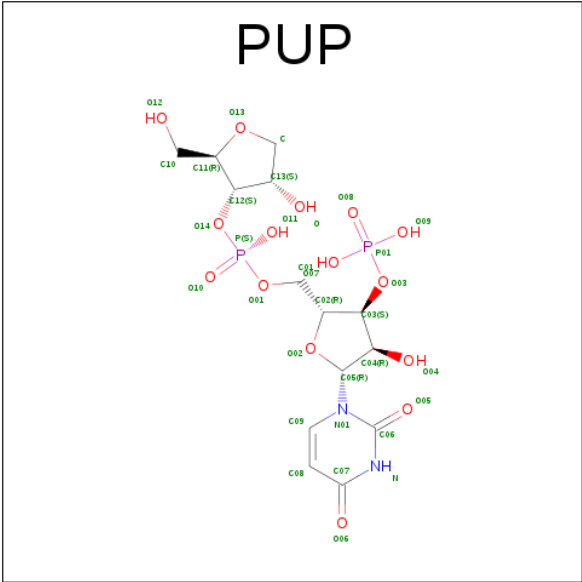


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is (2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-4-HYDROXY-2-({[(S)-HYDROXY{[(2R,3S,4S)-4-HYDROXY-2-(HYDROXYMETHYL)TETRAHYDROFURAN-3-YL]OXY}PHOSPHORYL]OXY}METHYL)TETRAHYDROFURAN-3-YL DIHYDROGEN PHOSPHATE (three-letter code: PUP) (formula: $C_{14}H_{22}N_2O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			33	14	2	15	2		

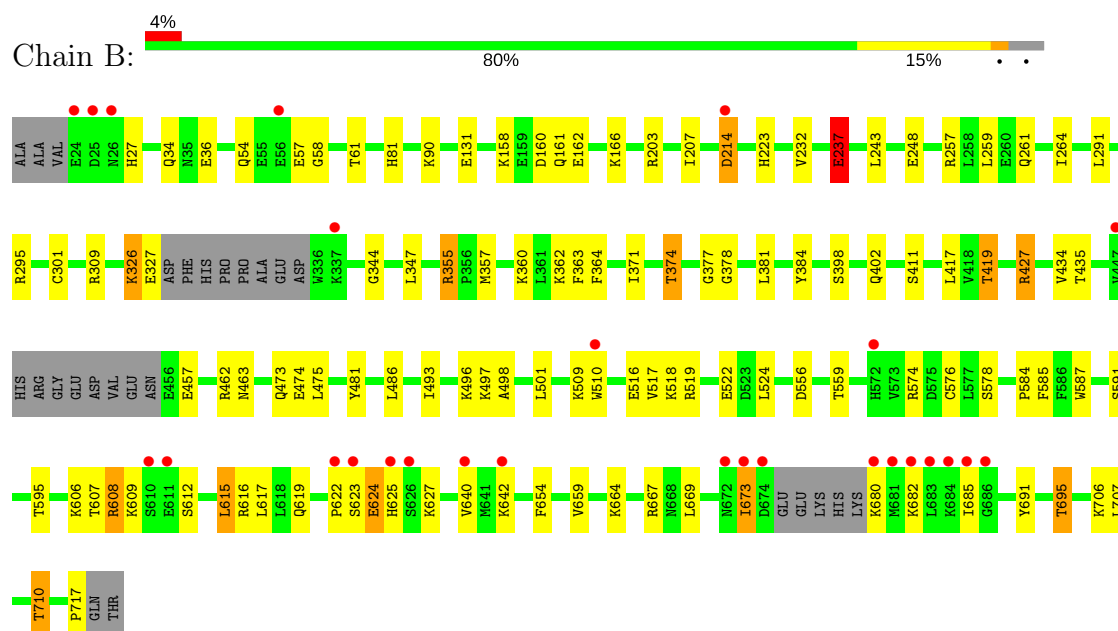
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	433	Total	O	0	0
			433	433		
6	A	15	Total	O	0	0
			15	15		
6	D	446	Total	O	0	0
			446	446		
6	C	17	Total	O	0	0
			17	17		

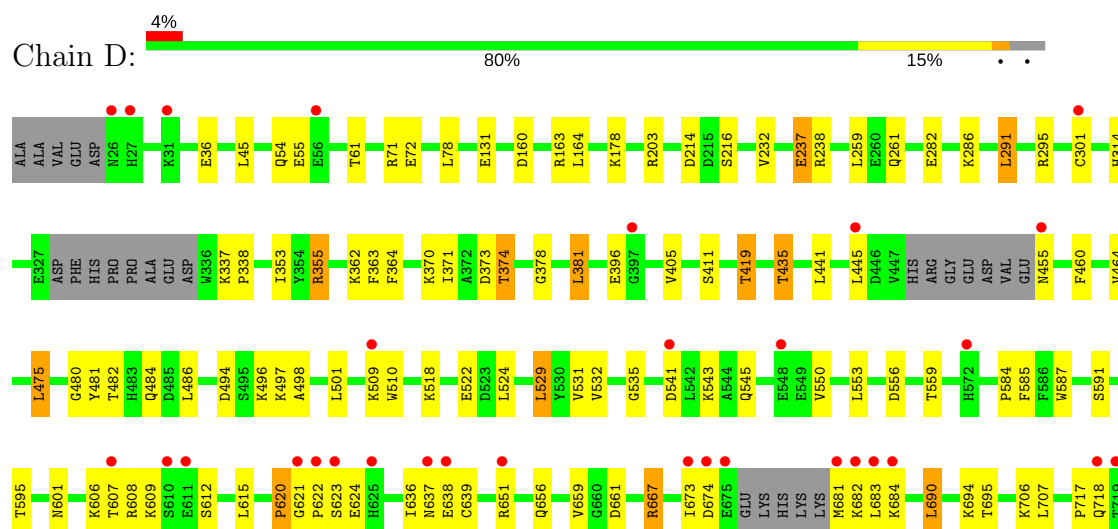
3 Residue-property plots

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

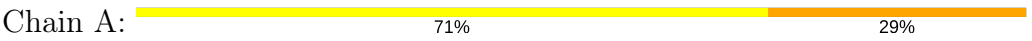
• Molecule 1: PROTEIN (RNase L)



• Molecule 1: PROTEIN (RNase L)



• Molecule 2: RNA (5'-R(P*(PO4)P*(PO4)P*AP*AP*AP*AP*(PO4))-2')



● Molecule 2: RNA (5'-R(P*(PO4)P*(PO4)P*AP*AP*AP*AP*(PO4))-2')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.61Å 160.70Å 230.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 2.10 46.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.62-2.10) 100.0 (46.62-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.229 0.198 , 0.229	Depositor DCC
R_{free} test set	6404 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11963	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.34 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8155e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, ACP, PUP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.25	0/5469	0.45	0/7362
1	D	0.25	0/5476	0.46	1/7373 (0.0%)
2	A	4.59	19/96 (19.8%)	6.47	44/140 (31.4%)
2	C	4.56	20/96 (20.8%)	6.49	40/140 (28.6%)
All	All	0.65	39/11137 (0.4%)	0.99	85/15015 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6	A	C6-N6	18.07	1.48	1.33
2	C	6	A	C6-N6	17.87	1.48	1.33
2	C	5	A	C6-N6	17.10	1.47	1.33
2	A	5	A	C6-N6	17.02	1.47	1.33
2	A	3	A	C6-N6	15.57	1.46	1.33
2	C	3	A	C6-N6	15.01	1.46	1.33
2	A	4	A	C6-N6	10.63	1.42	1.33
2	C	4	A	C6-N6	10.19	1.42	1.33
2	C	3	A	C3'-C2'	-9.01	1.42	1.52
2	A	4	A	C4'-C3'	-8.65	1.43	1.53
2	A	3	A	C3'-C2'	-8.60	1.43	1.52
2	C	4	A	C4'-C3'	-8.28	1.44	1.53
2	A	5	A	C3'-C2'	-8.27	1.43	1.52
2	A	4	A	C3'-C2'	-8.17	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	A	C3'-C2'	-7.97	1.44	1.52
2	C	4	A	C3'-C2'	-7.96	1.44	1.52
2	C	6	A	C3'-C2'	-7.72	1.44	1.52
2	C	6	A	C8-N7	7.65	1.36	1.31
2	A	6	A	C8-N7	7.25	1.36	1.31
2	A	6	A	C4'-C3'	-6.97	1.45	1.53
2	A	6	A	C3'-C2'	-6.96	1.45	1.52
2	C	6	A	C4'-C3'	-6.91	1.45	1.53
2	A	3	A	C4'-C3'	-6.87	1.45	1.53
2	C	3	A	C4'-C3'	-6.67	1.45	1.53
2	C	4	A	C8-N7	6.48	1.36	1.31
2	A	4	A	C8-N7	6.36	1.35	1.31
2	A	5	A	N3-C4	5.88	1.38	1.34
2	C	5	A	N7-C5	-5.61	1.35	1.39
2	A	6	A	C5-C4	5.61	1.42	1.38
2	C	3	A	C8-N7	5.49	1.35	1.31
2	C	5	A	C4'-C3'	-5.39	1.47	1.52
2	A	5	A	N7-C5	-5.36	1.36	1.39
2	C	6	A	C2'-C1'	-5.34	1.47	1.53
2	C	6	A	C5-C4	5.33	1.42	1.38
2	C	3	A	P-O5'	-5.30	1.54	1.59
2	C	5	A	N3-C4	5.23	1.38	1.34
2	A	3	A	P-O5'	-5.21	1.54	1.59
2	A	3	A	C8-N7	5.16	1.35	1.31
2	A	5	A	C4'-C3'	-5.13	1.47	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	A	C2-N3-C4	22.61	121.91	110.60
2	A	6	A	C2-N3-C4	20.98	121.09	110.60
2	A	4	A	C2-N3-C4	20.82	121.01	110.60
2	A	3	A	C2-N3-C4	20.78	120.99	110.60
2	C	5	A	C2-N3-C4	20.77	120.98	110.60
2	C	4	A	C2-N3-C4	20.69	120.95	110.60
2	C	6	A	C2-N3-C4	20.63	120.92	110.60
2	A	5	A	C2-N3-C4	20.59	120.89	110.60
2	C	5	A	N1-C2-N3	-18.89	119.85	129.30
2	A	5	A	N1-C2-N3	-18.55	120.03	129.30
2	A	4	A	N1-C2-N3	-17.88	120.36	129.30
2	C	4	A	N1-C2-N3	-17.60	120.50	129.30
2	C	3	A	N1-C2-N3	-17.39	120.60	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6	A	N1-C2-N3	-16.79	120.90	129.30
2	A	3	A	N1-C2-N3	-16.61	120.99	129.30
2	C	6	A	N1-C2-N3	-16.38	121.11	129.30
2	A	4	A	N3-C4-C5	-11.72	118.59	126.80
2	C	4	A	N3-C4-C5	-11.69	118.62	126.80
2	A	4	A	OP1-P-OP2	-11.46	102.41	119.60
2	C	3	A	N3-C4-C5	-11.32	118.88	126.80
2	C	3	A	OP1-P-OP2	-11.25	102.73	119.60
2	A	3	A	OP1-P-OP2	-11.13	102.90	119.60
2	C	4	A	OP1-P-OP2	-11.11	102.94	119.60
2	A	6	A	N3-C4-C5	-10.89	119.18	126.80
2	A	3	A	N3-C4-C5	-10.86	119.20	126.80
2	C	6	A	N3-C4-C5	-10.67	119.33	126.80
2	C	3	A	N7-C8-N9	-10.65	108.48	113.80
2	A	5	A	OP1-P-OP2	-10.56	103.76	119.60
2	A	3	A	N7-C8-N9	-10.38	108.61	113.80
2	A	5	A	N3-C4-C5	-9.90	119.87	126.80
2	C	5	A	OP1-P-OP2	-9.86	104.81	119.60
2	C	3	A	C5-N7-C8	9.81	108.80	103.90
2	A	3	A	C5-N7-C8	9.73	108.77	103.90
2	C	5	A	N3-C4-C5	-9.53	120.13	126.80
2	C	5	A	N7-C8-N9	-9.52	109.04	113.80
2	A	5	A	N7-C8-N9	-9.27	109.17	113.80
2	C	6	A	N7-C8-N9	-9.20	109.20	113.80
2	C	4	A	N7-C8-N9	-9.12	109.24	113.80
2	C	4	A	C5-N7-C8	9.01	108.40	103.90
2	A	4	A	N7-C8-N9	-8.89	109.35	113.80
2	C	5	A	C5-N7-C8	8.79	108.29	103.90
2	A	4	A	C5-N7-C8	8.76	108.28	103.90
2	C	6	A	C5-N7-C8	8.73	108.27	103.90
2	A	6	A	N3-C4-N9	8.67	134.33	127.40
2	A	5	A	C5-N7-C8	8.45	108.13	103.90
2	A	6	A	N7-C8-N9	-8.41	109.59	113.80
2	C	3	A	N3-C4-N9	8.28	134.02	127.40
2	A	3	A	N3-C4-N9	8.26	134.00	127.40
2	A	6	A	C5-N7-C8	8.23	108.02	103.90
2	C	6	A	N3-C4-N9	8.11	133.89	127.40
2	A	4	A	N3-C4-N9	8.10	133.88	127.40
2	C	4	A	N3-C4-N9	7.93	133.74	127.40
2	C	4	A	C4-C5-N7	-7.76	106.82	110.70
2	A	5	A	N3-C4-N9	7.62	133.49	127.40
2	C	3	A	C4-C5-N7	-7.52	106.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	A	C6-N1-C2	7.41	123.04	118.60
2	A	4	A	C4-C5-N7	-7.39	107.01	110.70
2	A	3	A	C8-N9-C4	7.34	108.74	105.80
2	A	3	A	C4-C5-N7	-7.22	107.09	110.70
2	C	3	A	C8-N9-C4	7.20	108.68	105.80
2	C	5	A	C6-N1-C2	7.05	122.83	118.60
2	A	5	A	C8-N9-C4	6.90	108.56	105.80
2	C	5	A	C4-C5-N7	-6.86	107.27	110.70
2	C	5	A	N3-C4-N9	6.79	132.83	127.40
2	C	4	A	C6-N1-C2	6.73	122.64	118.60
2	C	6	A	OP1-P-OP2	-6.72	109.51	119.60
2	C	6	A	C4-C5-N7	-6.71	107.35	110.70
2	A	4	A	C4-C5-C6	6.62	120.31	117.00
2	A	5	A	C6-N1-C2	6.55	122.53	118.60
2	C	6	A	C8-N9-C4	6.52	108.41	105.80
2	C	4	A	C4-C5-C6	6.50	120.25	117.00
2	C	5	A	C8-N9-C4	6.40	108.36	105.80
2	A	5	A	C4-C5-N7	-6.38	107.51	110.70
2	A	6	A	OP1-P-OP2	-6.13	110.41	119.60
2	A	6	A	C8-N9-C4	6.09	108.23	105.80
2	A	6	A	C4-C5-N7	-6.07	107.67	110.70
2	A	6	A	C3'-C2'-C1'	6.03	106.32	101.50
2	A	4	A	N1-C6-N6	5.97	122.18	118.60
2	A	6	A	C4'-C3'-C2'	5.83	108.43	102.60
1	D	509	LYS	N-CA-C	5.54	125.96	111.00
2	C	4	A	N1-C6-N6	5.50	121.90	118.60
2	A	5	A	O4'-C1'-N9	5.35	112.48	108.20
2	C	4	A	C8-N9-C4	5.26	107.90	105.80
2	A	4	A	C8-N9-C4	5.08	107.83	105.80
2	A	3	A	C5-C6-N6	-5.03	119.67	123.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	624	GLU	Peptide

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	B	5372	0	5377	77	0
1	D	5379	0	5381	80	0
2	A	101	0	44	8	0
2	C	101	0	44	4	0
3	B	31	0	14	1	0
3	D	31	0	14	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	D	33	0	19	3	0
6	A	15	0	0	3	0
6	B	433	0	0	20	0
6	C	17	0	0	1	0
6	D	446	0	0	16	0
All	All	11963	0	10893	162	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 7.

All (162) 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:B:309:ARG:NH1	1:B:327:GLU:OE2	1.91	1.03
2:A:6:A:OP2	6:A:111:HOH:O	1.85	0.94
1:D:261:GLN:OE1	6:D:1138:HOH:O	1.86	0.94
1:D:532:VAL:O	6:D:1249:HOH:O	1.87	0.92
1:B:248:GLU:OE1	6:B:1170:HOH:O	1.87	0.91
1:D:606:LYS:NZ	6:D:1475:HOH:O	2.04	0.90
1:D:639:CYS:HB3	1:D:684:LYS:HZ1	1.41	0.84
1:D:237:GLU:OE2	6:D:1505:HOH:O	1.97	0.83
1:B:411:SER:OG	6:B:988:HOH:O	2.01	0.76
2:A:7:PO4:O4	6:A:108:HOH:O	2.05	0.74
1:B:232:VAL:HG11	1:B:261:GLN:HG3	1.68	0.74
1:B:624:GLU:OE2	1:B:706:LYS:NZ	2.21	0.74
1:D:639:CYS:HB3	1:D:684:LYS:NZ	2.02	0.73
1:D:674:ASP:OD2	6:D:1507:HOH:O	2.06	0.73
1:D:282:GLU:OE2	6:D:1440:HOH:O	2.04	0.73
1:B:595:THR:HG21	1:B:717:PRO:HD3	1.69	0.72
1:D:624:GLU:OE2	1:D:706:LYS:NZ	2.21	0.71
1:B:160:ASP:OD2	6:B:1227:HOH:O	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ARG:NH1	1:D:237:GLU:OE1	2.21	0.71
5:D:1004:PUP:O06	6:D:1128:HOH:O	2.09	0.70
1:D:301:CYS:O	6:D:1235:HOH:O	2.09	0.69
1:D:72:GLU:OE2	6:D:1203:HOH:O	2.10	0.69
1:B:357:MET:SD	6:B:995:HOH:O	2.51	0.69
1:B:578:SER:OG	6:B:998:HOH:O	2.10	0.69
2:C:1:PO4:O3	6:C:105:HOH:O	2.11	0.69
2:A:1:PO4:O3	6:A:106:HOH:O	2.12	0.68
1:B:203:ARG:NH2	2:C:1:PO4:O3	2.26	0.68
1:B:519:ARG:NH1	6:B:1323:HOH:O	2.24	0.67
1:B:474:GLU:OE2	6:B:1239:HOH:O	2.12	0.66
1:D:411:SER:OG	6:D:1155:HOH:O	2.15	0.65
1:D:214:ASP:OD2	1:D:216:SER:OG	2.15	0.64
2:A:1:PO4:O3	1:D:203:ARG:NH2	2.31	0.63
1:D:374:THR:HB	1:D:378:GLY:HA2	1.80	0.63
1:D:595:THR:HG21	1:D:717:PRO:HD3	1.81	0.63
1:B:237:GLU:O	6:B:1035:HOH:O	2.16	0.62
1:D:607:THR:O	1:D:609:LYS:N	2.31	0.62
1:B:680:LYS:NZ	6:B:1206:HOH:O	2.21	0.62
1:B:642:LYS:NZ	6:B:1196:HOH:O	2.24	0.61
1:D:480:GLY:O	1:D:510:TRP:N	2.34	0.60
1:B:344:GLY:HA2	1:B:347:LEU:HB2	1.83	0.60
1:B:259:LEU:HD13	1:B:295:ARG:HG3	1.84	0.59
1:B:669:LEU:HD21	1:B:685:ILE:HD13	1.85	0.59
1:B:625:HIS:HB2	1:B:627:LYS:HG2	1.84	0.59
1:D:556:ASP:OD1	1:D:559:THR:HG23	2.03	0.59
1:D:232:VAL:HG11	1:D:261:GLN:HG3	1.85	0.58
1:D:673:ILE:HG23	1:D:682:LYS:HG2	1.86	0.58
1:D:591:SER:O	1:D:595:THR:HG23	2.03	0.58
1:D:690:LEU:HD22	1:D:694:LYS:HG3	1.84	0.58
1:B:609:LYS:HB3	1:B:612:SER:HB2	1.84	0.58
1:B:496:LYS:HB2	1:B:498:ALA:H	1.68	0.57
2:A:6:A:O3'	1:D:55:GLU:OE2	2.22	0.57
1:B:591:SER:O	1:B:595:THR:HG23	2.05	0.57
1:B:559:THR:HG22	1:B:585:PHE:CE1	2.40	0.56
1:D:496:LYS:N	1:D:497:LYS:HA	2.20	0.56
1:B:496:LYS:N	1:B:497:LYS:HA	2.21	0.56
1:B:377:GLY:O	1:D:163:ARG:NH1	2.38	0.56
1:B:607:THR:O	1:B:609:LYS:N	2.38	0.56
1:B:559:THR:HG22	1:B:585:PHE:HE1	1.72	0.56
1:D:45:LEU:HD11	1:D:78:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:GLU:HB3	1:D:71:ARG:NH1	2.22	0.55
1:D:659:VAL:HG23	6:D:1256:HOH:O	2.05	0.55
1:D:636:ILE:HG22	1:D:637:ASN:H	1.70	0.55
1:B:214:ASP:OD1	1:B:214:ASP:N	2.39	0.55
1:B:355:ARG:HD2	1:B:364:PHE:HB2	1.87	0.55
1:B:673:ILE:HG12	1:B:682:LYS:HG2	1.89	0.55
1:B:556:ASP:OD1	1:B:559:THR:HG23	2.07	0.54
1:B:90:LYS:HG3	6:B:1223:HOH:O	2.06	0.54
1:D:36:GLU:OE2	1:D:71:ARG:HD3	2.08	0.54
1:B:301:CYS:O	6:B:950:HOH:O	2.18	0.53
1:D:559:THR:HG22	1:D:585:PHE:CE1	2.43	0.53
1:B:510:TRP:HZ3	1:B:516:GLU:HB2	1.73	0.53
1:B:54:GLN:HG2	1:B:61:THR:HG22	1.89	0.53
1:D:54:GLN:HG2	1:D:61:THR:HG22	1.89	0.53
1:D:529:LEU:HD12	1:D:550:VAL:HG13	1.90	0.53
1:D:496:LYS:H	1:D:497:LYS:HA	1.74	0.53
1:D:601:ASN:OD1	1:D:667:ARG:NH1	2.39	0.52
1:B:496:LYS:H	1:B:497:LYS:HA	1.74	0.52
1:B:457:GLU:OE2	1:B:462:ARG:NH2	2.42	0.52
1:B:34:GLN:HE22	2:C:6:A:H2	1.57	0.52
1:D:718:GLN:NE2	6:D:1443:HOH:O	2.41	0.51
1:B:158:LYS:NZ	6:B:909:HOH:O	2.42	0.51
1:B:161:GLN:HG3	1:B:166:LYS:HD3	1.92	0.51
1:D:656:GLN:HG2	1:D:661:ASP:OD2	2.10	0.51
1:B:617:LEU:HD11	1:B:710:THR:HG21	1.93	0.50
1:D:355:ARG:HD2	1:D:364:PHE:HB2	1.94	0.50
1:D:559:THR:HG22	1:D:585:PHE:HE1	1.74	0.50
1:D:419:THR:H	1:D:435:THR:CG2	2.25	0.50
1:D:637:ASN:OD1	1:D:684:LYS:NZ	2.37	0.50
1:B:518:LYS:O	1:B:522:GLU:HG2	2.13	0.49
1:D:355:ARG:HB2	1:D:362:LYS:HE3	1.95	0.49
1:B:574:ARG:NH1	6:B:1165:HOH:O	2.34	0.49
1:D:259:LEU:HD12	1:D:291:LEU:HD13	1.95	0.49
1:D:371:ILE:HD11	1:D:381:LEU:HD13	1.93	0.49
1:B:419:THR:HG23	1:B:435:THR:OG1	2.13	0.49
1:B:659:VAL:HG23	6:B:1242:HOH:O	2.12	0.48
1:D:518:LYS:O	1:D:522:GLU:HG2	2.14	0.48
1:B:223:HIS:HE1	6:B:1264:HOH:O	1.97	0.48
1:D:510:TRP:HD1	6:D:1142:HOH:O	1.96	0.48
1:B:608:ARG:NH2	1:B:654:PHE:O	2.45	0.47
1:B:493:ILE:CG2	1:B:497:LYS:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:LYS:HB2	1:D:498:ALA:H	1.79	0.47
1:D:396:GLU:O	6:D:1171:HOH:O	2.20	0.47
1:B:131:GLU:OE2	2:C:3:A:N1	2.47	0.47
1:D:482:THR:HG21	1:D:484:GLN:HE21	1.79	0.47
1:D:475:LEU:HD22	1:D:481:TYR:HB2	1.97	0.47
1:D:622:PRO:HA	1:D:623:SER:HA	1.49	0.47
3:D:1001:ACP:H8	3:D:1001:ACP:O5'	2.15	0.47
1:D:651:ARG:NH1	5:D:1004:PUP:H11	2.29	0.47
1:B:691:TYR:O	1:B:695:THR:HG23	2.15	0.46
1:D:612:SER:OG	1:D:615:LEU:HB2	2.15	0.46
1:B:398:SER:O	1:B:402:GLN:HG2	2.16	0.46
1:B:326:LYS:H	1:B:326:LYS:HG3	1.45	0.46
1:D:419:THR:H	1:D:435:THR:HG23	1.80	0.46
1:B:427:ARG:NH1	2:A:1:PO4:O4	2.50	0.45
1:B:58:GLY:N	6:B:1223:HOH:O	2.33	0.45
3:B:801:ACP:H8	3:B:801:ACP:O5'	2.15	0.45
1:B:355:ARG:HB2	1:B:362:LYS:HE3	1.98	0.45
1:D:460:PHE:O	1:D:464:VAL:HG12	2.17	0.45
1:B:473:GLN:OE1	1:B:578:SER:OG	2.25	0.45
1:B:510:TRP:CZ3	1:B:517:VAL:HG23	2.52	0.45
1:D:259:LEU:HD22	1:D:295:ARG:HG2	1.99	0.45
1:B:622:PRO:HA	1:B:623:SER:HA	1.55	0.45
1:D:620:PRO:HB2	1:D:621:GLY:H	1.65	0.44
1:D:441:LEU:HD21	1:D:531:VAL:HG22	1.99	0.44
1:D:609:LYS:HB3	1:D:612:SER:HB3	1.97	0.44
1:B:309:ARG:NE	6:B:1009:HOH:O	2.40	0.44
1:D:445:LEU:HD13	1:D:535:GLY:HA3	2.00	0.44
1:D:370:LYS:NZ	1:D:373:ASP:OD1	2.40	0.44
1:B:584:PRO:HA	1:B:587:TRP:CG	2.53	0.44
1:D:178:LYS:HD3	1:D:178:LYS:HA	1.85	0.43
1:B:374:THR:HB	1:B:378:GLY:HA2	2.00	0.43
1:B:481:TYR:CZ	1:B:509:LYS:HD3	2.54	0.43
1:B:669:LEU:O	1:B:673:ILE:HB	2.19	0.43
1:D:482:THR:HB	6:D:1142:HOH:O	2.17	0.43
1:B:57:GLU:HG2	1:D:353:ILE:CG2	2.49	0.43
1:D:337:LYS:HD2	1:D:338:PRO:HD2	2.00	0.43
1:D:651:ARG:HH12	5:D:1004:PUP:H11	1.82	0.43
1:D:541:ASP:O	1:D:545:GLN:HG2	2.19	0.43
1:B:616:ARG:O	1:B:619:GLN:HG2	2.19	0.42
1:B:81:HIS:HE1	6:B:954:HOH:O	2.02	0.42
1:B:203:ARG:HG2	1:B:207:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:NH2	6:B:1009:HOH:O	2.48	0.42
1:B:584:PRO:HA	1:B:587:TRP:CD2	2.55	0.42
1:D:441:LEU:O	1:D:445:LEU:HG	2.20	0.42
1:B:243:LEU:HB2	1:B:264:ILE:HD11	2.02	0.42
1:B:357:MET:SD	1:B:362:LYS:HB2	2.60	0.42
2:A:2:PO4:O1	2:A:3:A:H5''	2.20	0.42
1:D:482:THR:HG21	1:D:484:GLN:NE2	2.35	0.42
1:D:683:LEU:HD23	1:D:683:LEU:HA	1.92	0.42
2:A:3:A:N1	1:D:131:GLU:OE2	2.53	0.42
1:B:360:LYS:HB3	1:B:384:TYR:O	2.19	0.41
1:B:617:LEU:O	1:B:706:LYS:HG3	2.20	0.41
1:D:482:THR:HG22	1:D:484:GLN:HG2	2.02	0.41
1:B:36:GLU:OE1	1:D:314:HIS:HE1	2.04	0.41
1:D:160:ASP:OD1	1:D:163:ARG:NH2	2.54	0.41
1:D:584:PRO:HA	1:D:587:TRP:CG	2.56	0.41
1:D:595:THR:CG2	1:D:717:PRO:HD3	2.49	0.41
1:B:371:ILE:HD11	1:B:381:LEU:HD13	2.01	0.41
1:D:543:LYS:HB3	1:D:543:LYS:HE2	1.86	0.41
1:B:606:LYS:HA	1:B:664:LYS:HD3	2.03	0.41
1:B:615:LEU:HA	1:B:615:LEU:HD12	1.84	0.40
1:D:595:THR:HG22	6:D:1496:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	665/699 (95%)	638 (96%)	25 (4%)	2 (0%)	44	44
1	D	666/699 (95%)	638 (96%)	25 (4%)	3 (0%)	32	28
All	All	1331/1398 (95%)	1276 (96%)	50 (4%)	5 (0%)	38	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	608	ARG
1	D	608	ARG
1	D	620	PRO
1	D	238	ARG
1	B	237	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	585/607 (96%)	558 (95%)	27 (5%)	31	29
1	D	586/607 (96%)	561 (96%)	25 (4%)	33	32
All	All	1171/1214 (96%)	1119 (96%)	52 (4%)	33	31

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	162	GLU
1	B	214	ASP
1	B	237	GLU
1	B	257	ARG
1	B	291	LEU
1	B	326	LYS
1	B	355	ARG
1	B	363	PHE
1	B	374	THR
1	B	417	LEU
1	B	419	THR
1	B	427	ARG
1	B	434	VAL
1	B	463	ASN
1	B	475	LEU
1	B	486	LEU
1	B	501	LEU

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Mol	Chain	Res	Type
1	B	524	LEU
1	B	576	CYS
1	B	615	LEU
1	B	640	VAL
1	B	667	ARG
1	B	673	ILE
1	B	695	THR
1	B	707	LEU
1	B	710	THR
1	D	164	LEU
1	D	237	GLU
1	D	286	LYS
1	D	291	LEU
1	D	355	ARG
1	D	363	PHE
1	D	374	THR
1	D	381	LEU
1	D	405	VAL
1	D	419	THR
1	D	435	THR
1	D	455	ASN
1	D	475	LEU
1	D	486	LEU
1	D	494	ASP
1	D	501	LEU
1	D	524	LEU
1	D	529	LEU
1	D	553	LEU
1	D	638	GLU
1	D	667	ARG
1	D	681	MET
1	D	690	LEU
1	D	695	THR
1	D	707	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	D	314	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	0/7	-	-
2	C	0/7	-	-
All	All	0/14	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	ACP	B	801	4	27,33,33	1.69	7 (25%)	30,52,52	2.22	8 (26%)
3	ACP	D	1001	4	27,33,33	1.69	6 (22%)	30,52,52	2.23	8 (26%)
5	PUP	D	1004	-	31,35,35	2.35	10 (32%)	38,53,53	1.66	5 (13%)

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	ACP	B	801	4	-	0/15/38/38	0/3/3/3
3	ACP	D	1001	4	-	0/15/38/38	0/3/3/3
5	PUP	D	1004	-	-	0/18/51/51	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1004	PUP	C04-C03	-5.03	1.41	1.53
5	D	1004	PUP	C13-C12	-4.55	1.44	1.53
5	D	1004	PUP	C04-C05	-4.41	1.46	1.53
3	D	1001	ACP	C2'-C1'	-3.92	1.47	1.53
3	D	1001	ACP	C2'-C3'	-3.84	1.43	1.53
3	B	801	ACP	C2'-C1'	-3.82	1.47	1.53
3	B	801	ACP	C2'-C3'	-3.81	1.43	1.53
5	D	1004	PUP	C-C13	-3.41	1.46	1.51
5	D	1004	PUP	O13-C11	-2.78	1.39	1.44
3	B	801	ACP	PB-O2B	-2.67	1.49	1.56
3	D	1001	ACP	C3'-C4'	-2.58	1.46	1.53
3	D	1001	ACP	PB-O2B	-2.55	1.50	1.56
3	B	801	ACP	C3'-C4'	-2.51	1.46	1.53
5	D	1004	PUP	O02-C02	-2.50	1.39	1.45
5	D	1004	PUP	C12-C11	-2.45	1.46	1.52
5	D	1004	PUP	O-C13	-2.19	1.38	1.43
3	B	801	ACP	PG-O2G	-2.09	1.50	1.54
3	D	1001	ACP	O4'-C4'	-2.06	1.40	1.45
3	B	801	ACP	C4-N3	2.06	1.38	1.35
5	D	1004	PUP	C07-N	2.20	1.37	1.33
3	B	801	ACP	C6-N6	2.44	1.44	1.34
3	D	1001	ACP	C6-N6	2.50	1.44	1.34
5	D	1004	PUP	O06-C07	6.62	1.41	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ACP	N3-C2-N1	-9.12	120.91	128.86
3	D	1001	ACP	N3-C2-N1	-8.98	121.04	128.86
3	D	1001	ACP	O3G-PG-O1G	-2.87	104.62	112.32
3	B	801	ACP	O3G-PG-O1G	-2.61	105.33	112.32
3	D	1001	ACP	PA-O3A-PB	-2.60	124.02	132.39
3	B	801	ACP	O2G-PG-O1G	-2.54	105.51	112.32
3	D	1001	ACP	O2G-PG-O1G	-2.47	105.71	112.32
3	B	801	ACP	C4-C5-N7	-2.44	107.05	109.41
3	D	1001	ACP	C4-C5-N7	-2.42	107.07	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1004	PUP	C02-O02-C05	-2.29	107.33	109.77
3	B	801	ACP	PA-O3A-PB	-2.22	125.25	132.39
3	B	801	ACP	O2B-PB-O1B	-2.18	102.80	110.09
3	D	1001	ACP	O2B-PB-O1B	-2.01	103.35	110.09
5	D	1004	PUP	C-C13-C12	2.40	104.74	101.88
3	D	1001	ACP	O2G-PG-C3B	2.52	112.51	106.40
5	D	1004	PUP	O01-C01-C02	2.79	118.91	109.00
3	B	801	ACP	O2G-PG-C3B	2.80	113.20	106.40
3	B	801	ACP	O3G-PG-C3B	2.99	113.65	106.40
3	D	1001	ACP	O3G-PG-C3B	3.29	114.38	106.40
5	D	1004	PUP	O02-C05-N01	3.47	115.03	108.08
5	D	1004	PUP	C07-N-C06	7.56	120.62	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	ACP	1	0
3	D	1001	ACP	1	0
5	D	1004	PUP	3	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, 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	B	673/699 (96%)	0.03	27 (4%) 39 46	33, 53, 92, 136	0
1	D	674/699 (96%)	0.02	31 (4%) 33 39	34, 54, 89, 130	0
2	A	4/7 (57%)	-0.59	0 100 100	43, 45, 45, 102	0
2	C	4/7 (57%)	-0.51	0 100 100	40, 41, 44, 97	0
All	All	1355/1412 (95%)	0.02	58 (4%) 36 43	33, 54, 92, 136	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	683	LEU	8.8
1	D	683	LEU	7.1
1	B	623	SER	6.8
1	B	626	SER	6.0
1	B	682	LYS	5.9
1	D	623	SER	5.8
1	D	455	ASN	5.5
1	B	685	ILE	5.3
1	D	625	HIS	5.2
1	B	625	HIS	4.9
1	B	622	PRO	4.7
1	B	681	MET	4.5
1	D	682	LYS	4.3
1	B	680	LYS	4.1
1	D	637	ASN	3.6
1	B	672	ASN	3.1
1	D	611	GLU	3.1
1	D	607	THR	3.1
1	B	611	GLU	3.1
1	D	509	LYS	3.0
1	D	572	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	56	GLU	2.9
1	D	610	SER	2.9
1	B	510	TRP	2.8
1	D	301	CYS	2.8
1	D	622	PRO	2.8
1	D	684	LYS	2.8
1	D	548	GLU	2.7
1	D	674	ASP	2.6
1	B	673	ILE	2.6
1	D	651	ARG	2.6
1	B	24	GLU	2.6
1	D	718	GLN	2.6
1	D	719	THR	2.5
1	B	337	LYS	2.5
1	D	26	ASN	2.5
1	B	572	HIS	2.5
1	B	25	ASP	2.5
1	B	610	SER	2.4
1	D	397	GLY	2.4
1	D	675	GLU	2.4
1	D	445	LEU	2.3
1	B	684	LYS	2.3
1	D	27	HIS	2.3
1	B	674	ASP	2.3
1	D	56	GLU	2.3
1	D	31	LYS	2.2
1	B	640	VAL	2.2
1	D	638	GLU	2.2
1	B	447	VAL	2.2
1	D	541	ASP	2.1
1	B	642	LYS	2.1
1	B	686	GLY	2.1
1	D	621	GLY	2.1
1	D	673	ILE	2.0
1	B	26	ASN	2.0
1	D	681	MET	2.0
1	B	214	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	PUP	D	1004	33/33	0.89	0.15	0.11	58,87,103,107	0
4	MG	D	1003	1/1	0.99	0.09	-0.28	48,48,48,48	0
3	ACP	D	1001	31/31	0.98	0.10	-0.66	40,47,65,77	0
3	ACP	B	801	31/31	0.97	0.09	-1.01	41,46,57,68	0
4	MG	B	803	1/1	0.99	0.06	-2.69	48,48,48,48	0
4	MG	D	1002	1/1	0.97	0.03	-	47,47,47,47	0
4	MG	B	802	1/1	0.97	0.07	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.