



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 AM GMT

PDB ID : 2JLV
Title : DENGUE VIRUS 4 NS3 HELICASE IN COMPLEX WITH SSRNA AND AMPPNP
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Deposited on : 2008-09-15
Resolution : 1.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

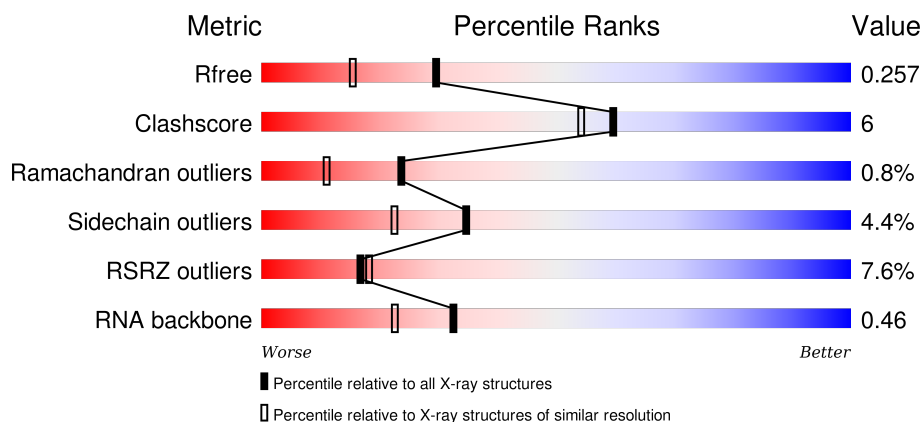
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)
RNA backbone	2183	1028 (2.70-1.10)

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	A	451	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	451	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
2	C	12	<div> <div>25%</div> <div>25%</div> <div>8%</div> <div>42%</div> </div>
2	D	12	<div> <div>17%</div> <div>33%</div> <div>8%</div> <div>42%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8294 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 SERINE PROTEASE SUBUNIT NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	2	0
			3622	2282	647	675	18			
1	B	451	Total	C	N	O	S	0	2	0
			3622	2282	647	675	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	GLU	CONFLICT	UNP Q2YHF0
A	292	CYS	SER	CONFLICT	UNP Q2YHF0
A	321	SER	THR	CONFLICT	UNP Q2YHF0
A	322	ILE	THR	CONFLICT	UNP Q2YHF0
A	381	ARG	LYS	CONFLICT	UNP Q2YHF0
A	480	LYS	ARG	CONFLICT	UNP Q2YHF0
B	250	ASP	GLU	CONFLICT	UNP Q2YHF0
B	292	CYS	SER	CONFLICT	UNP Q2YHF0
B	321	SER	THR	CONFLICT	UNP Q2YHF0
B	322	ILE	THR	CONFLICT	UNP Q2YHF0
B	381	ARG	LYS	CONFLICT	UNP Q2YHF0
B	480	LYS	ARG	CONFLICT	UNP Q2YHF0

- Molecule 2 is a RNA chain called 5'-R(*AP*GP*AP*CP*UP*AP*AP*CP*AP*AP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	0	0	0
			128	58	20	44	6			
2	D	7	Total	C	N	O	P	0	0	0
			128	58	20	44	6			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

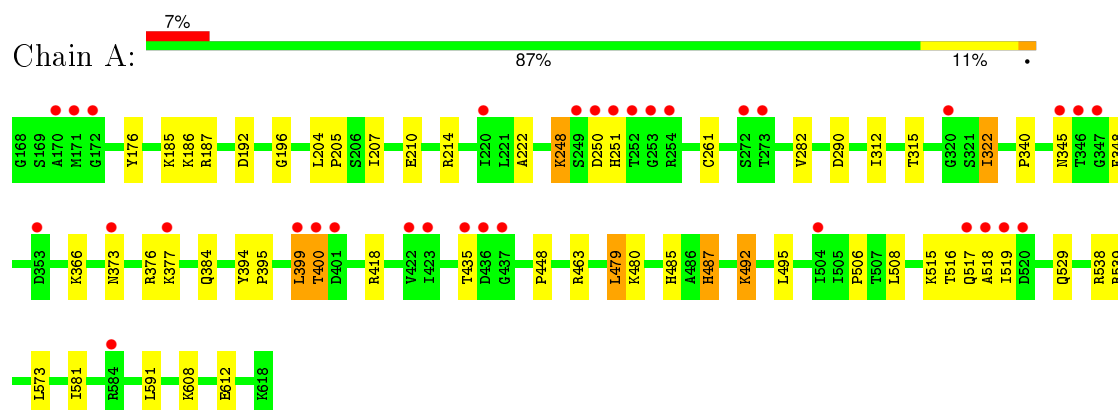
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	349	Total O 349 349	0	0
7	B	339	Total O 339 339	0	0
7	C	17	Total O 17 17	0	0
7	D	11	Total O 11 11	0	0

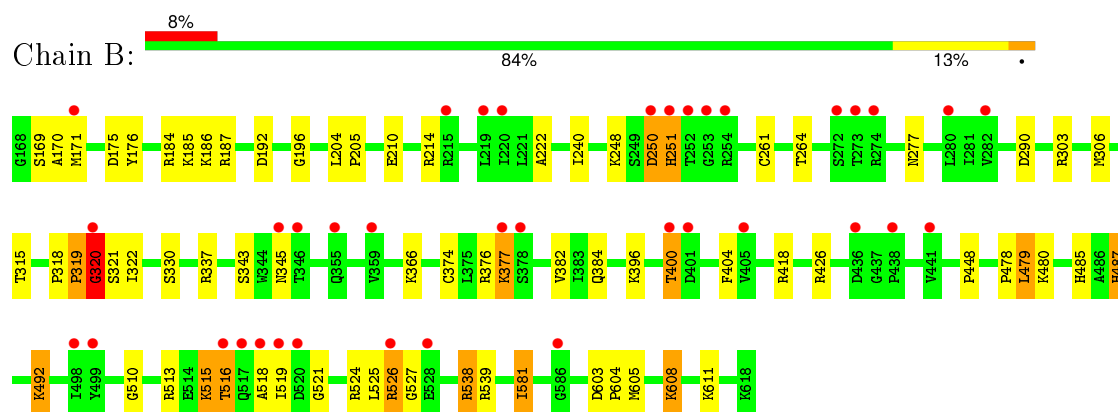
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

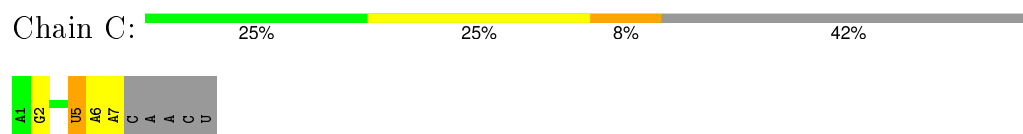
• Molecule 1: SERINE PROTEASE SUBUNIT NS3



• Molecule 1: SERINE PROTEASE SUBUNIT NS3



• Molecule 2: 5'-R(*AP*GP*AP*CP*UP*AP*AP*CP*AP*AP*CP*U)-3'



• Molecule 2: 5'-R(*AP*GP*AP*CP*UP*AP*AP*CP*AP*AP*CP*U)-3'





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.66 Å 105.19 Å 72.44 Å 90.00° 117.66° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-1.90) 87.2 (19.83-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.248 0.202 , 0.257	Depositor DCC
R_{free} test set	3104 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60736 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8294	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MN, ANP, CL

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	0.48	0/3703	0.62	2/5011 (0.0%)
1	B	0.46	0/3703	0.62	1/5011 (0.0%)
2	C	0.69	0/142	1.36	1/219 (0.5%)
2	D	0.64	0/142	1.27	1/219 (0.5%)
All	All	0.48	0/7690	0.67	5/10460 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	LEU	C-N-CA	6.20	137.20	121.70
1	A	399	LEU	N-CA-C	5.73	126.47	111.00
2	C	5	U	O4'-C1'-N1	5.43	112.55	108.20
1	B	515	LYS	C-N-CA	5.32	134.99	121.70
2	D	5	U	O4'-C1'-N1	5.31	112.44	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	GLY	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	A	3622	0	3613	38	1
1	B	3622	0	3613	48	1
2	C	128	0	68	1	0
2	D	128	0	68	3	0
3	A	31	0	13	2	0
3	B	31	0	13	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	8	2	0
5	B	6	0	8	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	349	0	0	4	0
7	B	339	0	0	2	0
7	C	17	0	0	0	0
7	D	11	0	0	0	0
All	All	8294	0	7404	85	1

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 6.

All (85) 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:250:ASP:HB3	1:A:251:HIS:HA	1.32	1.11
1:A:518:ALA:CB	1:A:519:ILE:HA	1.81	1.11
1:A:176:TYR:HB2	5:A:1621:GOL:H32	1.31	1.11
1:B:250:ASP:HA	1:B:251:HIS:HB3	1.32	1.08
1:B:518:ALA:HB1	1:B:519:ILE:HA	1.37	1.04
1:A:518:ALA:HB1	1:A:519:ILE:HA	1.03	1.03
1:A:518:ALA:HB1	1:A:519:ILE:CA	1.93	0.98
1:B:176:TYR:HB3	5:B:1621:GOL:O3	1.65	0.96
1:B:196:GLY:H	3:B:1619:ANP:HNB1	1.15	0.90
1:A:250:ASP:CB	1:A:251:HIS:HA	2.05	0.86
1:B:376:ARG:HH22	1:B:384:GLN:HE21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HD11	1:A:506:PRO:HB2	1.61	0.81
1:B:250:ASP:HA	1:B:251:HIS:CB	2.13	0.76
1:A:399:LEU:N	1:A:400:THR:OG1	2.20	0.74
1:A:196:GLY:H	3:A:1619:ANP:HNB1	1.39	0.71
1:B:518:ALA:HB1	1:B:519:ILE:CA	2.17	0.70
1:A:250:ASP:HB3	1:A:251:HIS:CA	2.17	0.68
1:B:171[A]:MET:HG3	1:B:171[A]:MET:O	1.94	0.68
1:A:581:ILE:HD13	1:A:591:LEU:HB2	1.77	0.66
1:B:290:ASP:OD1	2:D:2:G:N2	2.30	0.64
1:B:176:TYR:CB	5:B:1621:GOL:O3	2.45	0.62
1:B:492:LYS:HG3	7:B:2237:HOH:O	2.00	0.61
1:A:376:ARG:HH22	1:A:384:GLN:HE21	1.48	0.61
1:A:250:ASP:CB	1:A:251:HIS:CA	2.77	0.61
1:B:526:ARG:H	1:B:526:ARG:HE	1.49	0.60
1:B:185:LYS:O	1:B:186:LYS:HB2	2.01	0.59
1:A:176:TYR:CB	5:A:1621:GOL:H32	2.19	0.58
1:B:222:ALA:O	1:B:261:CYS:HA	2.03	0.58
1:A:448:PRO:HB2	1:A:479:LEU:HB2	1.87	0.56
1:B:516:THR:N	7:B:2258:HOH:O	2.38	0.56
1:B:303:ARG:HA	1:B:306:MET:HE2	1.87	0.56
1:B:176:TYR:HB3	5:B:1621:GOL:HO3	1.68	0.56
1:A:518:ALA:CB	1:A:519:ILE:CA	2.63	0.55
1:B:319:PRO:O	1:B:320:GLY:C	2.45	0.55
1:A:492:LYS:HE2	1:A:492:LYS:HA	1.91	0.52
1:B:581:ILE:HD11	1:B:611:LYS:HG2	1.91	0.52
1:B:448:PRO:HB2	1:B:479:LEU:HB2	1.91	0.52
1:B:277:ASN:OD1	1:B:303:ARG:NH2	2.42	0.52
1:A:185:LYS:O	1:A:186:LYS:HB2	2.09	0.51
1:B:192:ASP:HA	1:B:315:THR:O	2.11	0.50
1:B:521:GLY:O	1:B:524:ARG:HG2	2.11	0.50
1:A:192:ASP:HA	1:A:315:THR:O	2.11	0.50
1:A:480:LYS:HE3	7:A:2242:HOH:O	2.12	0.49
1:B:322:ILE:HG22	1:B:480:LYS:HD3	1.96	0.48
1:B:426:ARG:NH1	1:B:478:PRO:HD3	2.28	0.48
1:B:525:LEU:HD23	1:B:526:ARG:HH11	1.78	0.48
1:B:538:ARG:NH1	2:D:4:C:O2	2.46	0.48
1:B:604:PRO:O	1:B:608:LYS:NZ	2.45	0.47
1:A:210:GLU:O	1:A:214:ARG:HG3	2.15	0.46
1:B:396:LYS:O	1:B:400:THR:HB	2.14	0.46
1:A:322:ILE:H	1:A:322:ILE:HD12	1.81	0.46
1:B:210:GLU:O	1:B:214:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LYS:N	1:B:516:THR:O	2.49	0.46
1:B:169:SER:HB3	1:B:175:ASP:HA	1.98	0.46
1:B:322:ILE:CG2	1:B:480:LYS:HD3	2.45	0.45
1:B:608:LYS:HA	1:B:608:LYS:HD3	1.67	0.45
1:A:222:ALA:O	1:A:261:CYS:HA	2.16	0.45
1:A:248:LYS:HE2	1:B:248:LYS:HE3	1.98	0.45
1:A:290:ASP:OD1	2:C:2:G:N2	2.50	0.44
1:A:394:TYR:N	1:A:395:PRO:HD2	2.32	0.44
1:B:196:GLY:N	3:B:1619:ANP:HNB1	1.98	0.44
1:A:612:GLU:HG2	7:A:2338:HOH:O	2.17	0.44
1:A:340:PRO:HD3	1:A:348:PHE:CE1	2.52	0.44
1:B:184:ARG:O	1:B:187:ARG:HB3	2.16	0.44
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.99	0.43
1:B:374:CYS:O	1:B:377:LYS:HE3	2.18	0.43
1:B:382:VAL:HG22	1:B:404:PHE:HB2	1.99	0.43
1:A:516:THR:HG22	1:A:517:GLN:N	2.33	0.43
1:B:204:LEU:HB3	1:B:205:PRO:HD3	2.00	0.43
1:B:318:PRO:O	1:B:320:GLY:N	2.51	0.43
1:A:207:ILE:HD13	1:A:312:ILE:HD13	2.01	0.42
1:A:463:ARG:HH12	3:A:1619:ANP:HNB1	1.66	0.42
1:A:581:ILE:CD1	1:A:591:LEU:HB2	2.47	0.42
1:B:518:ALA:CB	1:B:519:ILE:HA	2.17	0.42
1:B:480:LYS:HE2	1:B:480:LYS:HB3	1.82	0.42
1:A:485:HIS:CE1	1:A:487:HIS:CD2	3.07	0.42
1:B:170[A]:ALA:O	1:B:171[A]:MET:HB3	2.19	0.42
1:A:204:LEU:HD13	1:A:282:VAL:HG11	2.02	0.42
1:A:529:GLN:NE2	7:A:2276:HOH:O	2.52	0.42
1:A:492:LYS:HE3	1:A:508:LEU:HG	2.01	0.41
1:B:485:HIS:CE1	1:B:487:HIS:CD2	3.08	0.41
1:B:603:ASP:OD2	1:B:605:MET:HB2	2.21	0.40
1:A:539:ARG:HD2	7:A:2281:HOH:O	2.20	0.40
1:B:264:THR:OG1	2:D:5:U:H5'	2.21	0.40
1:B:250:ASP:CA	1:B:251:HIS:CB	2.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH1	1:B:513:ARG:O[1_556]	2.08	0.12

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	451/451 (100%)	435 (96%)	15 (3%)	1 (0%)	52	42
1	B	451/451 (100%)	427 (95%)	18 (4%)	6 (1%)	15	4
All	All	902/902 (100%)	862 (96%)	33 (4%)	7 (1%)	24	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	THR
1	B	320	GLY
1	B	251	HIS
1	B	527	GLY
1	B	319	PRO
1	B	516	THR
1	B	510	GLY

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	389/388 (100%)	374 (96%)	15 (4%)	39	27
1	B	389/388 (100%)	370 (95%)	19 (5%)	31	18
All	All	778/776 (100%)	744 (96%)	34 (4%)	35	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	A	322	ILE
1	A	345	ASN
1	A	366	LYS
1	A	373	ASN
1	A	377	LYS
1	A	418	ARG
1	A	435	THR
1	A	479	LEU
1	A	487	HIS
1	A	492	LYS
1	A	515	LYS
1	A	538	ARG
1	A	573	LEU
1	A	608	LYS
1	B	240	ILE
1	B	250	ASP
1	B	321	SER
1	B	330	SER
1	B	337	ARG
1	B	343	SER
1	B	345	ASN
1	B	366	LYS
1	B	377	LYS
1	B	400	THR
1	B	418	ARG
1	B	479	LEU
1	B	487	HIS
1	B	492	LYS
1	B	526	ARG
1	B	538	ARG
1	B	539	ARG
1	B	581	ILE
1	B	608	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	345	ASN
1	A	384	GLN
1	A	467	GLN
1	A	487	HIS

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Mol	Chain	Res	Type
1	A	529	GLN
1	B	279	ASN
1	B	345	ASN
1	B	384	GLN
1	B	467	GLN
1	B	487	HIS
1	B	529	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	6/12 (50%)	2 (33%)	1 (16%)
2	D	6/12 (50%)	2 (33%)	0
All	All	12/24 (50%)	4 (33%)	1 (8%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	A
2	C	7	A
2	D	6	A
2	D	7	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	5	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ANP	A	1619	4	27,33,33	2.01	6 (22%)	30,52,52	2.36	5 (16%)
5	GOL	A	1621	-	5,5,5	0.20	0	5,5,5	0.66	0
3	ANP	B	1619	4	27,33,33	1.92	5 (18%)	30,52,52	2.07	6 (20%)
5	GOL	B	1621	-	5,5,5	0.44	0	5,5,5	0.47	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	ANP	A	1619	4	-	0/12/38/38	0/3/3/3
5	GOL	A	1621	-	-	0/4/4/4	0/0/0/0
3	ANP	B	1619	4	-	0/12/38/38	0/3/3/3
5	GOL	B	1621	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1619	ANP	PB-O3A	2.09	1.61	1.59
3	B	1619	ANP	C5-C4	3.02	1.47	1.40
3	A	1619	ANP	C5-C4	3.15	1.47	1.40
3	B	1619	ANP	PB-O1B	3.75	1.50	1.46
3	A	1619	ANP	PB-N3B	3.81	1.73	1.63
3	A	1619	ANP	PG-N3B	3.85	1.73	1.63
3	B	1619	ANP	PB-N3B	3.93	1.73	1.63
3	A	1619	ANP	PG-O1G	4.01	1.50	1.46
3	B	1619	ANP	PG-N3B	4.06	1.74	1.63
3	B	1619	ANP	PG-O1G	4.32	1.51	1.46
3	A	1619	ANP	PB-O1B	5.29	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1619	ANP	N3-C2-N1	-8.10	122.69	128.89
3	A	1619	ANP	N3-C2-N1	-7.76	122.95	128.89
3	A	1619	ANP	O1G-PG-N3B	-7.68	100.11	111.90
3	B	1619	ANP	O1B-PB-N3B	-2.81	107.58	111.90
3	A	1619	ANP	C4-C5-N7	-2.62	107.07	109.48
3	B	1619	ANP	C4-C5-N7	-2.48	107.20	109.48
3	B	1619	ANP	O1G-PG-N3B	-2.08	108.71	111.90
3	A	1619	ANP	O3A-PA-O5'	-2.06	97.46	102.94
3	B	1619	ANP	O2B-PB-O1B	2.97	116.20	110.00
3	B	1619	ANP	O3G-PG-O2G	2.98	116.42	107.58
3	A	1619	ANP	O2B-PB-O1B	3.47	117.24	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1619	ANP	2	0
5	A	1621	GOL	2	0
3	B	1619	ANP	2	0
5	B	1621	GOL	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	A	451/451 (100%)	0.76	33 (7%)	18 20	16, 23, 33, 42	0
1	B	451/451 (100%)	0.62	37 (8%)	14 16	12, 23, 33, 43	0
2	C	7/12 (58%)	0.18	0	100 100	21, 23, 33, 37	0
2	D	7/12 (58%)	0.22	0	100 100	19, 21, 32, 35	0
All	All	916/926 (98%)	0.68	70 (7%)	17 18	12, 23, 33, 43	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	ILE	6.8
1	A	249	SER	6.6
1	B	272	SER	6.6
1	A	250	ASP	6.4
1	A	400	THR	6.0
1	B	273	THR	5.9
1	A	519	ILE	5.6
1	A	273	THR	5.5
1	A	399	LEU	5.5
1	A	171[A]	MET	5.4
1	A	518	ALA	4.8
1	B	518	ALA	4.7
1	A	272	SER	4.6
1	B	254	ARG	4.4
1	B	171[A]	MET	4.3
1	B	250	ASP	4.1
1	A	345	ASN	4.1
1	B	252	THR	4.0
1	A	517	GLN	3.9
1	A	251	HIS	3.9
1	B	528	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	253	GLY	3.7
1	B	436	ASP	3.6
1	A	252	THR	3.5
1	B	517	GLN	3.5
1	B	516	THR	3.3
1	A	320	GLY	3.2
1	A	436	ASP	3.2
1	B	526	ARG	3.1
1	A	254	ARG	3.1
1	A	504	ILE	3.1
1	B	520	ASP	3.1
1	B	378	SER	3.1
1	A	346	THR	3.1
1	A	170[A]	ALA	3.0
1	B	400	THR	3.0
1	B	401	ASP	3.0
1	A	347	GLY	2.9
1	A	401	ASP	2.9
1	B	251	HIS	2.8
1	A	437	GLY	2.7
1	B	274	ARG	2.7
1	A	220	ILE	2.7
1	B	320	GLY	2.6
1	A	423	ILE	2.6
1	B	405	VAL	2.5
1	B	377	LYS	2.4
1	B	220	ILE	2.4
1	A	373	ASN	2.4
1	B	253	GLY	2.4
1	B	438	PRO	2.4
1	B	345	ASN	2.3
1	A	377	LYS	2.3
1	B	359	VAL	2.3
1	A	520	ASP	2.3
1	B	219	LEU	2.2
1	B	282	VAL	2.2
1	B	355	GLN	2.2
1	B	441	VAL	2.2
1	A	584	ARG	2.2
1	B	280	LEU	2.2
1	A	353	ASP	2.1
1	A	422	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	435	THR	2.1
1	B	346	THR	2.1
1	B	586	GLY	2.1
1	A	172	GLY	2.1
1	B	498	ILE	2.1
1	B	215	ARG	2.1
1	B	499	TYR	2.0

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

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(Å ²)	Q<0.9
5	GOL	A	1621	6/6	0.91	0.17	1.98	26,29,30,33	0
3	ANP	B	1619	31/31	0.95	0.13	0.07	15,26,33,33	0
3	ANP	A	1619	31/31	0.95	0.13	-0.06	12,23,32,32	0
5	GOL	B	1621	6/6	0.91	0.11	-0.49	32,33,34,34	0
4	MN	A	1620	1/1	0.98	0.04	-	14,14,14,14	0
4	MN	B	1620	1/1	0.99	0.04	-	18,18,18,18	0
6	CL	B	1622	1/1	0.99	0.05	-	23,23,23,23	0
6	CL	A	1622	1/1	0.97	0.10	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.