



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:25 AM GMT

PDB ID : 3PKM
Title : Crystal structure of Cas6 with its substrate RNA
Authors : Wang, R.; Preamplume, G.; Li, H.
Deposited on : 2010-11-11
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

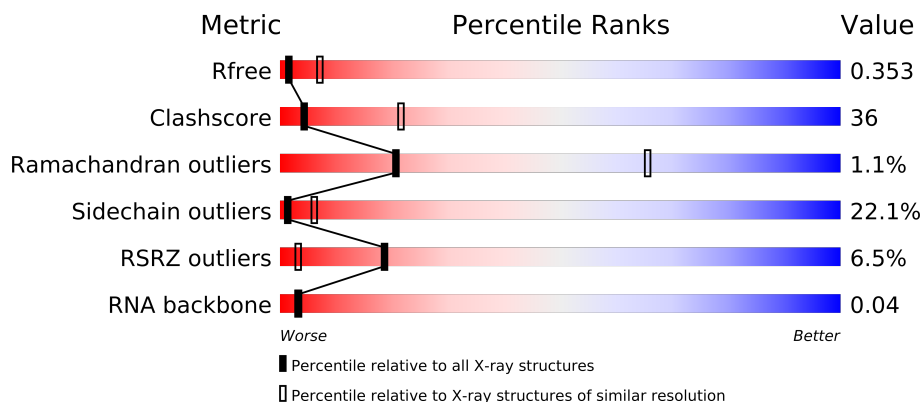
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance





The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	269	
1	X	269	
2	G	10	
3	R	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4195 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cas6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1891	1250	309	325	7			
1	X	233	Total	C	N	O	S	0	0	0
			1925	1270	318	330	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	EXPRESSION TAG	UNP Q8U1S4
A	3	HIS	-	EXPRESSION TAG	UNP Q8U1S4
A	4	HIS	-	EXPRESSION TAG	UNP Q8U1S4
A	5	HIS	-	EXPRESSION TAG	UNP Q8U1S4
A	6	GLY	-	EXPRESSION TAG	UNP Q8U1S4
A	7	SER	-	EXPRESSION TAG	UNP Q8U1S4
X	2	HIS	-	EXPRESSION TAG	UNP Q8U1S4
X	3	HIS	-	EXPRESSION TAG	UNP Q8U1S4
X	4	HIS	-	EXPRESSION TAG	UNP Q8U1S4
X	5	HIS	-	EXPRESSION TAG	UNP Q8U1S4
X	6	GLY	-	EXPRESSION TAG	UNP Q8U1S4
X	7	SER	-	EXPRESSION TAG	UNP Q8U1S4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			189	86	34	60	9			

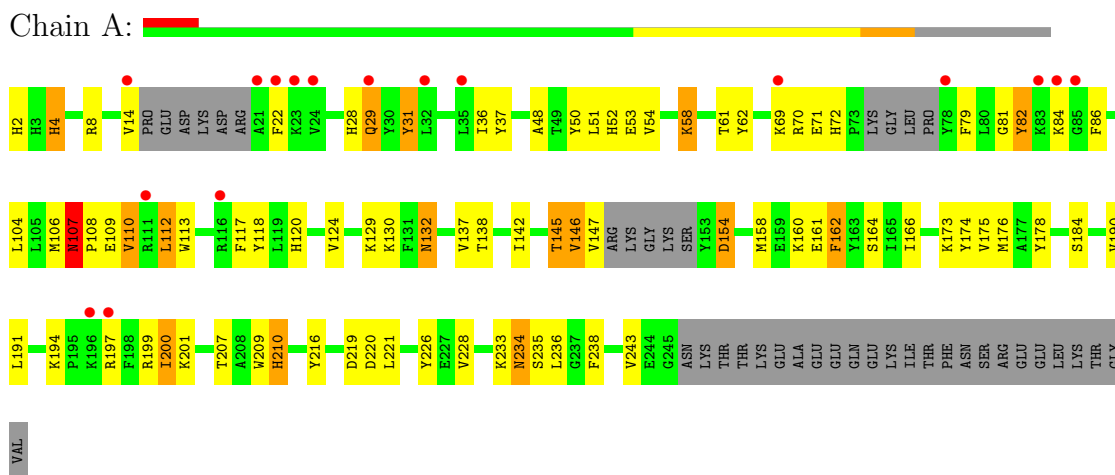
- Molecule 3 is a RNA chain called 5'-R(P*UP*UP*AP*CP*AP*AP*UP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	9	Total	C	N	O	P	0	0	0
			190	86	34	61	9			

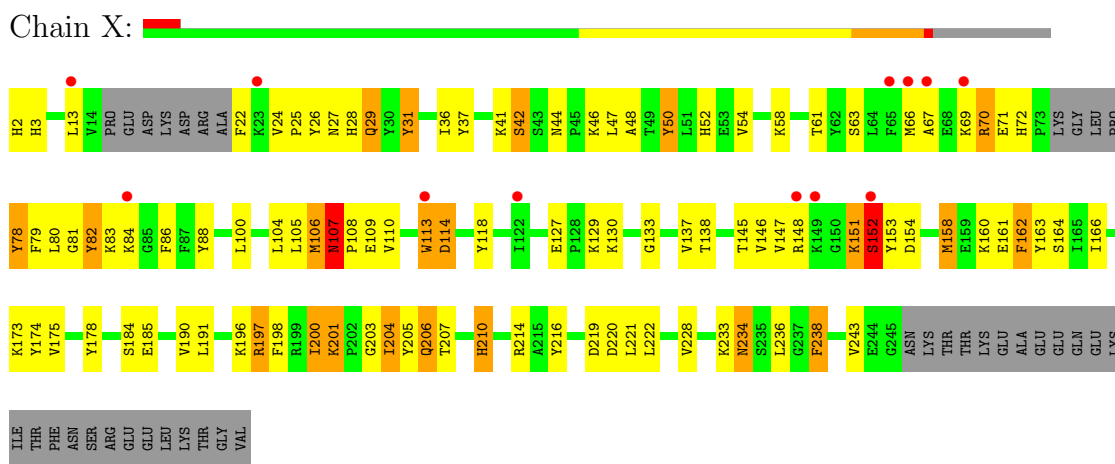
3 Residue-property plots

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: Cas6 protein



• Molecule 1: Cas6 protein



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



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

Chain R: 

U2	U3	A4	C5	A6	A7	U8	A9	A10
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.56Å 96.56Å 165.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.35 – 3.10 46.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	69.4 (46.35-3.10) 69.7 (46.35-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1.357)	Depositor
R, R_{free}	0.276 , 0.318 0.318 , 0.353	Depositor DCC
R_{free} test set	1201 reflections (10.33%)	DCC
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.9	EDS
Estimated twinning fraction	0.051 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14522 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4195	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.35	0/1948	0.68	2/2628 (0.1%)
1	X	0.41	0/1983	0.72	3/2673 (0.1%)
2	G	0.62	0/211	1.32	1/325 (0.3%)
3	R	0.70	0/212	1.40	4/327 (1.2%)
All	All	0.42	0/4354	0.80	10/5953 (0.2%)

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	X	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	107	ASN	C-N-CD	-5.86	107.70	120.60
1	A	107	ASN	C-N-CD	-5.82	107.80	120.60
3	R	5	C	C6-N1-C2	-5.70	118.02	120.30
3	R	10	A	C8-N9-C4	-5.70	103.52	105.80
1	X	152	SER	N-CA-C	5.56	126.02	111.00
3	R	10	A	N7-C8-N9	5.41	116.51	113.80
2	G	6	A	N9-C4-C5	-5.33	103.67	105.80
1	X	220	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	220	ASP	CB-CG-OD2	5.20	122.98	118.30
3	R	6	A	N7-C8-N9	5.12	116.36	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	42	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1891	0	0	48	0
1	X	1925	0	0	90	0
2	G	189	0	0	9	0
3	R	190	0	0	22	0
All	All	4195	0	0	151	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:107:ASN:CB	1:X:108:PRO:CD	2.43	0.97
1:A:107:ASN:CB	1:A:108:PRO:CD	2.43	0.96
1:X:197:ARG:NE	3:R:10:A:C8	2.43	0.86
1:X:197:ARG:NH2	1:X:205:TYR:CB	2.38	0.86
1:X:81:GLY:C	1:X:82:TYR:CD2	2.52	0.83
1:X:72:HIS:CE1	3:R:6:A:C1'	2.64	0.80
1:X:197:ARG:CZ	3:R:10:A:C8	2.65	0.80
1:X:151:LYS:CE	1:X:153:TYR:N	2.46	0.78
1:X:196:LYS:NZ	3:R:7:A:OP2	2.15	0.78
1:X:148:ARG:CD	1:X:152:SER:OG	2.34	0.76
1:X:151:LYS:NZ	1:X:205:TYR:OH	2.22	0.73
1:X:153:TYR:CB	3:R:10:A:N1	2.52	0.73
1:A:200:ILE:CD1	1:A:200:ILE:N	2.50	0.72
2:G:2:U:O2'	2:G:3:U:C5'	2.38	0.71
1:A:31:TYR:CE1	1:A:113:TRP:CZ3	2.79	0.71
1:X:152:SER:O	1:X:153:TYR:CG	2.44	0.70
3:R:2:U:O2'	3:R:3:U:OP2	2.10	0.70
1:X:197:ARG:NH2	3:R:10:A:C1'	2.55	0.69
1:X:69:LYS:CB	1:X:82:TYR:CE1	2.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:R:2:U:O2'	3:R:3:U:C5'	2.41	0.68
1:A:22:PHE:CE2	1:A:84:LYS:O	2.47	0.68
1:X:27:ASN:CA	1:X:198:PHE:CE2	2.77	0.67
1:A:31:TYR:CE1	1:A:113:TRP:CE3	2.83	0.67
2:G:2:U:O2'	2:G:3:U:OP2	2.12	0.66
2:G:2:U:C2'	2:G:3:U:OP2	2.44	0.66
3:R:2:U:C2'	3:R:3:U:OP2	2.43	0.66
1:A:120:HIS:O	1:X:105:LEU:CB	2.43	0.66
1:X:151:LYS:NZ	1:X:153:TYR:CA	2.60	0.65
1:X:29:GLN:OE1	1:X:238:PHE:CE1	2.50	0.65
1:X:29:GLN:CD	1:X:238:PHE:CE1	2.71	0.64
1:X:233:LYS:O	1:X:236:LEU:N	2.31	0.63
1:X:78:TYR:C	1:X:78:TYR:CD1	2.71	0.63
1:X:151:LYS:NZ	1:X:205:TYR:CE1	2.66	0.63
1:X:82:TYR:N	1:X:82:TYR:CD2	2.67	0.62
1:X:238:PHE:CD1	1:X:238:PHE:N	2.66	0.62
1:X:22:PHE:CE2	1:X:84:LYS:O	2.53	0.61
1:X:42:SER:O	1:X:42:SER:OG	2.17	0.60
1:A:112:LEU:CD1	1:A:117:PHE:CD2	2.85	0.60
1:X:198:PHE:N	1:X:206:GLN:O	2.35	0.60
1:X:13:LEU:O	1:X:84:LYS:CB	2.50	0.59
1:A:233:LYS:O	1:A:236:LEU:N	2.36	0.59
1:X:31:TYR:CD2	1:X:31:TYR:N	2.71	0.58
1:A:138:THR:OG1	1:A:210:HIS:ND1	2.36	0.58
1:X:205:TYR:CD2	1:X:205:TYR:N	2.73	0.56
1:X:151:LYS:CD	1:X:205:TYR:OH	2.54	0.56
1:A:31:TYR:CD2	1:A:31:TYR:N	2.72	0.56
1:X:67:ALA:O	3:R:5:C:N4	2.39	0.55
1:X:26:TYR:CG	3:R:7:A:C5	2.94	0.55
1:X:71:GLU:C	1:X:72:HIS:CD2	2.80	0.55
1:A:108:PRO:CB	1:A:110:VAL:N	2.70	0.55
1:X:63:SER:N	1:X:88:TYR:O	2.40	0.54
1:A:132:ASN:ND2	1:A:132:ASN:C	2.61	0.54
1:A:58:LYS:CD	1:A:58:LYS:N	2.69	0.54
1:A:51:LEU:O	1:A:54:VAL:O	2.26	0.53
1:X:70:ARG:C	1:X:82:TYR:OH	2.46	0.53
1:X:25:PRO:CD	1:X:113:TRP:CZ3	2.92	0.53
1:X:197:ARG:NH2	1:X:205:TYR:CG	2.77	0.52
1:A:2:HIS:ND1	1:A:4:HIS:CD2	2.77	0.52
1:X:203:GLY:O	1:X:204:ILE:CG1	2.57	0.52
1:X:154:ASP:OD1	1:X:207:THR:N	2.43	0.52
1:X:197:ARG:NH2	3:R:10:A:N9	2.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:71:GLU:N	1:X:82:TYR:OH	2.43	0.52
1:X:108:PRO:CB	1:X:110:VAL:N	2.73	0.52
1:X:197:ARG:NH2	3:R:10:A:C8	2.77	0.51
1:X:152:SER:O	1:X:153:TYR:CD1	2.62	0.51
3:R:2:U:O2'	3:R:3:U:P	2.69	0.51
2:G:8:U:C2'	2:G:9:A:C8	2.93	0.51
1:A:71:GLU:C	1:A:72:HIS:CD2	2.84	0.51
1:X:26:TYR:CE1	3:R:7:A:C8	2.99	0.50
2:G:2:U:O2'	2:G:3:U:P	2.69	0.50
1:A:199:ARG:O	1:A:201:LYS:NZ	2.44	0.50
1:A:2:HIS:CD2	1:X:2:HIS:CD2	3.00	0.50
1:A:22:PHE:O	1:A:81:GLY:CA	2.60	0.50
3:R:8:U:C2'	3:R:9:A:C8	2.95	0.50
1:X:22:PHE:CZ	1:X:84:LYS:O	2.65	0.49
1:X:61:THR:CB	1:X:228:VAL:O	2.60	0.49
1:A:2:HIS:ND1	1:A:4:HIS:NE2	2.61	0.49
1:X:80:LEU:O	1:X:82:TYR:CE2	2.66	0.49
1:X:151:LYS:NZ	1:X:205:TYR:CZ	2.81	0.49
1:X:66:MET:CE	1:X:88:TYR:CE1	2.96	0.49
1:X:206:GLN:NE2	1:X:206:GLN:CA	2.76	0.48
1:A:69:LYS:CB	1:A:82:TYR:CE1	2.96	0.48
1:X:50:TYR:C	1:X:50:TYR:CD2	2.86	0.48
1:X:151:LYS:CE	1:X:153:TYR:CA	2.91	0.48
1:A:71:GLU:O	1:A:79:PHE:CB	2.62	0.48
1:X:197:ARG:NH2	1:X:205:TYR:CD1	2.82	0.47
1:X:148:ARG:NH1	1:X:152:SER:OG	2.46	0.47
1:X:29:GLN:OE1	1:X:238:PHE:CZ	2.67	0.47
1:X:31:TYR:CD1	1:X:113:TRP:CB	2.97	0.47
1:A:61:THR:CB	1:A:228:VAL:O	2.63	0.47
1:X:24:VAL:O	1:X:79:PHE:N	2.47	0.47
1:A:154:ASP:OD1	1:A:207:THR:N	2.48	0.47
1:X:148:ARG:N	1:X:152:SER:CB	2.78	0.47
1:X:26:TYR:CD2	3:R:7:A:C4	3.03	0.46
1:A:48:ALA:O	1:A:52:HIS:CD2	2.68	0.46
1:X:108:PRO:CA	1:X:109:GLU:CB	2.93	0.46
1:A:108:PRO:CA	1:A:109:GLU:CB	2.93	0.46
1:X:162:PHE:CD2	1:X:162:PHE:C	2.89	0.46
1:X:26:TYR:CE1	1:X:79:PHE:CD1	3.04	0.46
1:X:72:HIS:N	1:X:72:HIS:CD2	2.84	0.45
1:A:8:ARG:NH2	1:A:226:TYR:O	2.49	0.45
1:A:201:LYS:CD	1:A:201:LYS:N	2.79	0.45
1:X:148:ARG:CD	1:X:152:SER:CB	2.94	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:27:ASN:C	1:X:198:PHE:CE2	2.90	0.45
1:X:200:ILE:O	1:X:201:LYS:CB	2.64	0.45
1:X:204:ILE:CG2	1:X:205:TYR:N	2.80	0.45
1:A:22:PHE:CD1	1:A:22:PHE:C	2.91	0.45
1:A:173:LYS:NZ	1:A:234:ASN:OD1	2.50	0.45
1:A:112:LEU:CD1	1:A:117:PHE:CE2	2.99	0.44
1:A:146:VAL:CG1	1:A:147:VAL:N	2.80	0.44
1:X:36:ILE:CG2	1:X:37:TYR:N	2.80	0.44
1:X:63:SER:OG	1:X:88:TYR:N	2.50	0.44
1:X:173:LYS:NZ	1:X:234:ASN:OD1	2.50	0.44
1:A:238:PHE:CD1	1:A:238:PHE:N	2.85	0.44
1:A:82:TYR:CD1	1:A:82:TYR:N	2.85	0.44
2:G:4:A:C5'	2:G:5:C:O5'	2.65	0.44
1:A:194:LYS:NZ	2:G:6:A:OP1	2.51	0.44
1:X:146:VAL:CG1	1:X:147:VAL:N	2.81	0.43
1:X:133:GLY:O	1:X:214:ARG:NH2	2.51	0.43
1:A:62:TYR:N	1:A:62:TYR:CD1	2.86	0.43
1:X:138:THR:OG1	1:X:210:HIS:ND1	2.51	0.43
1:A:2:HIS:O	1:A:2:HIS:CD2	2.71	0.43
1:X:26:TYR:CE2	1:X:78:TYR:O	2.71	0.43
1:X:152:SER:C	1:X:153:TYR:CG	2.92	0.43
1:X:26:TYR:CD2	3:R:7:A:C5	3.06	0.43
1:A:29:GLN:OE1	1:A:238:PHE:CE1	2.72	0.42
1:X:26:TYR:CB	3:R:7:A:C6	3.02	0.42
1:X:174:TYR:O	1:X:178:TYR:N	2.52	0.42
1:A:174:TYR:O	1:A:178:TYR:N	2.52	0.42
3:R:4:A:C4'	3:R:5:C:O5'	2.68	0.42
2:G:4:A:O2'	2:G:5:C:OP2	2.38	0.42
1:A:2:HIS:O	1:A:2:HIS:CG	2.72	0.42
1:A:145:THR:CG2	1:A:154:ASP:OD2	2.68	0.42
1:A:142:ILE:O	1:A:209:TRP:N	2.53	0.42
1:X:158:MET:N	1:X:158:MET:SD	2.93	0.42
1:X:114:ASP:C	1:X:114:ASP:OD1	2.58	0.42
1:X:174:TYR:CZ	1:X:178:TYR:CD1	3.08	0.42
1:A:129:LYS:NZ	1:A:129:LYS:CB	2.83	0.42
3:R:4:A:O2'	3:R:5:C:OP2	2.37	0.41
2:G:4:A:C4'	2:G:5:C:O5'	2.67	0.41
1:X:163:TYR:N	1:X:163:TYR:CD2	2.88	0.41
1:A:36:ILE:CG2	1:A:37:TYR:N	2.82	0.41
1:A:233:LYS:O	1:A:235:SER:N	2.53	0.41
3:R:4:A:C5'	3:R:5:C:O5'	2.69	0.41
1:X:71:GLU:O	1:X:79:PHE:CD2	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:HIS:N	1:A:72:HIS:CD2	2.88	0.41
1:A:162:PHE:CD2	1:A:162:PHE:C	2.94	0.41
1:X:44:ASN:OD1	1:X:47:LEU:N	2.54	0.41
1:X:48:ALA:O	1:X:52:HIS:CD2	2.74	0.41
1:A:120:HIS:CD2	1:X:106:MET:CB	3.03	0.40
1:X:152:SER:C	1:X:153:TYR:CD1	2.95	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	A	221/269 (82%)	198 (90%)	21 (10%)	2 (1%)	25	71
1	X	227/269 (84%)	200 (88%)	24 (11%)	3 (1%)	18	60
All	All	448/538 (83%)	398 (89%)	45 (10%)	5 (1%)	21	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	X	107	ASN
1	X	204	ILE
1	A	234	ASN
1	X	234	ASN

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	A	202/238 (85%)	161 (80%)	41 (20%)	2	8
1	X	206/238 (87%)	157 (76%)	49 (24%)	1	4
All	All	408/476 (86%)	318 (78%)	90 (22%)	1	6

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	14	VAL
1	A	28	HIS
1	A	29	GLN
1	A	31	TYR
1	A	50	TYR
1	A	53	GLU
1	A	58	LYS
1	A	70	ARG
1	A	82	TYR
1	A	86	PHE
1	A	104	LEU
1	A	106	MET
1	A	110	VAL
1	A	112	LEU
1	A	118	TYR
1	A	124	VAL
1	A	130	LYS
1	A	132	ASN
1	A	137	VAL
1	A	145	THR
1	A	146	VAL
1	A	154	ASP
1	A	158	MET
1	A	160	LYS
1	A	161	GLU
1	A	162	PHE
1	A	164	SER
1	A	166	ILE
1	A	175	VAL
1	A	176	MET
1	A	184	SER
1	A	190	VAL
1	A	191	LEU
1	A	197	ARG

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Mol	Chain	Res	Type
1	A	200	ILE
1	A	210	HIS
1	A	216	TYR
1	A	219	ASP
1	A	221	LEU
1	A	243	VAL
1	X	3	HIS
1	X	28	HIS
1	X	29	GLN
1	X	31	TYR
1	X	41	LYS
1	X	46	LYS
1	X	50	TYR
1	X	54	VAL
1	X	58	LYS
1	X	70	ARG
1	X	78	TYR
1	X	82	TYR
1	X	83	LYS
1	X	86	PHE
1	X	100	LEU
1	X	104	LEU
1	X	106	MET
1	X	113	TRP
1	X	114	ASP
1	X	118	TYR
1	X	127	GLU
1	X	129	LYS
1	X	130	LYS
1	X	137	VAL
1	X	145	THR
1	X	151	LYS
1	X	152	SER
1	X	158	MET
1	X	160	LYS
1	X	161	GLU
1	X	162	PHE
1	X	164	SER
1	X	166	ILE
1	X	175	VAL
1	X	184	SER
1	X	185	GLU

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Mol	Chain	Res	Type
1	X	190	VAL
1	X	191	LEU
1	X	197	ARG
1	X	200	ILE
1	X	201	LYS
1	X	206	GLN
1	X	210	HIS
1	X	216	TYR
1	X	219	ASP
1	X	221	LEU
1	X	222	LEU
1	X	238	PHE
1	X	243	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	9/10 (90%)	7 (77%)	4 (44%)
3	R	9/9 (100%)	7 (77%)	4 (44%)
All	All	18/19 (94%)	14 (77%)	8 (44%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	3	U
2	G	4	A
2	G	5	C
2	G	6	A
2	G	7	A
2	G	8	U
2	G	10	A
3	R	3	U
3	R	4	A
3	R	5	C
3	R	6	A
3	R	7	A
3	R	8	U
3	R	10	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	2	U
2	G	3	U
2	G	4	A
2	G	6	A
3	R	2	U
3	R	3	U
3	R	4	A
3	R	6	A

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	229/269 (85%)	0.46	17 (7%)	14 2	83, 158, 220, 243	0
1	X	233/269 (86%)	0.36	12 (5%)	26 4	76, 160, 221, 257	0
2	G	9/10 (90%)	0.35	0	100 100	159, 211, 239, 251	0
3	R	9/9 (100%)	0.55	2 (22%)	1 0	165, 219, 249, 253	0
All	All	480/557 (86%)	0.41	31 (6%)	18 3	76, 161, 225, 257	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	5.2
1	A	69	LYS	4.3
1	X	67	ALA	3.7
1	A	85	GLY	3.7
1	X	66	MET	3.7
1	A	29	GLN	3.6
1	X	23	LYS	3.6
1	A	197	ARG	3.3
1	X	13	LEU	3.2
1	A	24	VAL	3.0
1	A	83	LYS	2.8
1	X	148	ARG	2.8
1	X	149	LYS	2.6
1	X	65	PHE	2.6
1	A	116	ARG	2.5
1	X	113	TRP	2.4
1	X	122	ILE	2.3
1	X	69	LYS	2.3
1	A	21	ALA	2.2
1	A	23	LYS	2.2
3	R	6	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	84	LYS	2.2
1	A	35	LEU	2.2
1	A	14	VAL	2.2
1	X	152	SER	2.1
3	R	10	A	2.1
1	A	22	PHE	2.1
1	A	32	LEU	2.1
1	A	84	LYS	2.1
1	A	111	ARG	2.1
1	A	78	TYR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.