Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:24 PM GMT

PDB ID	:	4LG2
Title	:	Crystal structure of Reston Ebola virus VP35 RNA binding domain bound to 12-bp dsRNA
Authors	:	Bale, S.; Julien, J-P.; Bornholdt, Z.A.; Krois, A.S.; Wilson, I.A.; Saphire. E.O.
Deposited on	:	2013-06-27
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

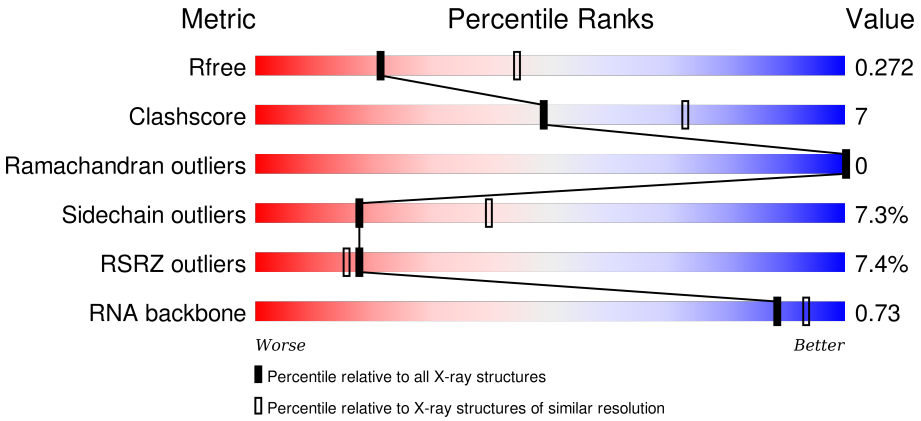
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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 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 <=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	146	% 65% 17% • 16%
1	B	146	68% 14% • 16%
1	C	146	12% 61% 21% • 16%
1	D	146	8% 68% 15% • 16%

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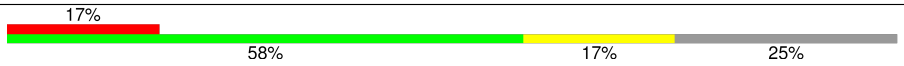
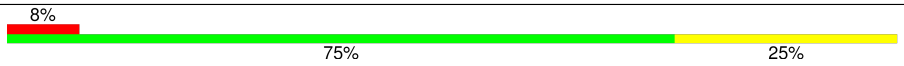
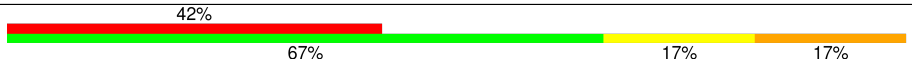
Mol	Chain	Length	Quality of chain
2	E	12	
2	F	12	
2	I	12	
2	J	12	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4703 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 Polymerase cofactor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	B	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	C	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			
1	D	122	Total	C	N	O	S	0	0	0
			952	609	169	168	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	MET	-	EXPRESSION TAG	UNP Q8JPY0
A	185	ALA	-	EXPRESSION TAG	UNP Q8JPY0
A	186	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	187	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	188	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	189	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	190	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	191	HIS	-	EXPRESSION TAG	UNP Q8JPY0
A	192	VAL	-	EXPRESSION TAG	UNP Q8JPY0
A	193	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	194	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	195	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	196	ASP	-	EXPRESSION TAG	UNP Q8JPY0
A	197	LYS	-	EXPRESSION TAG	UNP Q8JPY0
A	198	GLU	-	EXPRESSION TAG	UNP Q8JPY0
A	199	ASN	-	EXPRESSION TAG	UNP Q8JPY0
A	200	LEU	-	EXPRESSION TAG	UNP Q8JPY0
A	201	TYR	-	EXPRESSION TAG	UNP Q8JPY0
A	202	PHE	-	EXPRESSION TAG	UNP Q8JPY0
A	203	GLN	-	EXPRESSION TAG	UNP Q8JPY0
A	204	SER	-	EXPRESSION TAG	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	184	MET	-	EXPRESSION TAG	UNP Q8JPY0
B	185	ALA	-	EXPRESSION TAG	UNP Q8JPY0
B	186	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	187	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	188	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	189	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	190	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	191	HIS	-	EXPRESSION TAG	UNP Q8JPY0
B	192	VAL	-	EXPRESSION TAG	UNP Q8JPY0
B	193	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	194	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	195	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	196	ASP	-	EXPRESSION TAG	UNP Q8JPY0
B	197	LYS	-	EXPRESSION TAG	UNP Q8JPY0
B	198	GLU	-	EXPRESSION TAG	UNP Q8JPY0
B	199	ASN	-	EXPRESSION TAG	UNP Q8JPY0
B	200	LEU	-	EXPRESSION TAG	UNP Q8JPY0
B	201	TYR	-	EXPRESSION TAG	UNP Q8JPY0
B	202	PHE	-	EXPRESSION TAG	UNP Q8JPY0
B	203	GLN	-	EXPRESSION TAG	UNP Q8JPY0
B	204	SER	-	EXPRESSION TAG	UNP Q8JPY0
C	184	MET	-	EXPRESSION TAG	UNP Q8JPY0
C	185	ALA	-	EXPRESSION TAG	UNP Q8JPY0
C	186	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	187	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	188	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	189	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	190	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	191	HIS	-	EXPRESSION TAG	UNP Q8JPY0
C	192	VAL	-	EXPRESSION TAG	UNP Q8JPY0
C	193	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	194	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	195	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	196	ASP	-	EXPRESSION TAG	UNP Q8JPY0
C	197	LYS	-	EXPRESSION TAG	UNP Q8JPY0
C	198	GLU	-	EXPRESSION TAG	UNP Q8JPY0
C	199	ASN	-	EXPRESSION TAG	UNP Q8JPY0
C	200	LEU	-	EXPRESSION TAG	UNP Q8JPY0
C	201	TYR	-	EXPRESSION TAG	UNP Q8JPY0
C	202	PHE	-	EXPRESSION TAG	UNP Q8JPY0
C	203	GLN	-	EXPRESSION TAG	UNP Q8JPY0
C	204	SER	-	EXPRESSION TAG	UNP Q8JPY0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	184	MET	-	EXPRESSION TAG	UNP Q8JPY0
D	185	ALA	-	EXPRESSION TAG	UNP Q8JPY0
D	186	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	187	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	188	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	189	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	190	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	191	HIS	-	EXPRESSION TAG	UNP Q8JPY0
D	192	VAL	-	EXPRESSION TAG	UNP Q8JPY0
D	193	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	194	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	195	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	196	ASP	-	EXPRESSION TAG	UNP Q8JPY0
D	197	LYS	-	EXPRESSION TAG	UNP Q8JPY0
D	198	GLU	-	EXPRESSION TAG	UNP Q8JPY0
D	199	ASN	-	EXPRESSION TAG	UNP Q8JPY0
D	200	LEU	-	EXPRESSION TAG	UNP Q8JPY0
D	201	TYR	-	EXPRESSION TAG	UNP Q8JPY0
D	202	PHE	-	EXPRESSION TAG	UNP Q8JPY0
D	203	GLN	-	EXPRESSION TAG	UNP Q8JPY0
D	204	SER	-	EXPRESSION TAG	UNP Q8JPY0

- Molecule 2 is a RNA chain called dsRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	P	0	0	0
			187	85	33	61	8			
2	F	9	Total	C	N	O	P	0	0	0
			193	86	35	63	9			
2	J	12	Total	C	N	O	P	0	0	0
			255	114	45	84	12			
2	I	12	Total	C	N	O	P	0	0	0
			252	114	45	82	11			

- Molecule 3 is water.

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

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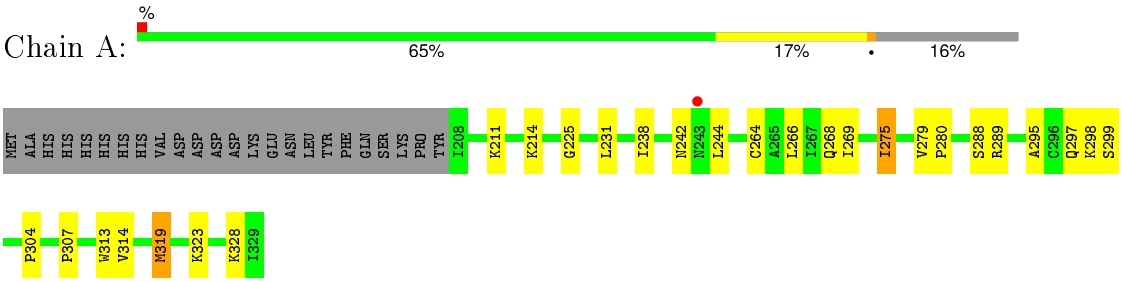
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

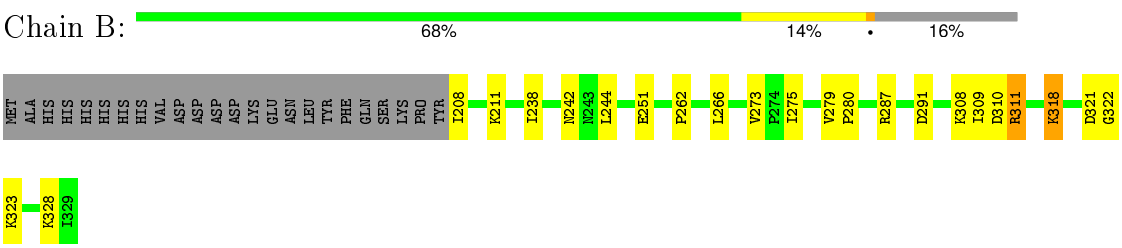
- Molecule 1: Polymerase cofactor

Chain A:



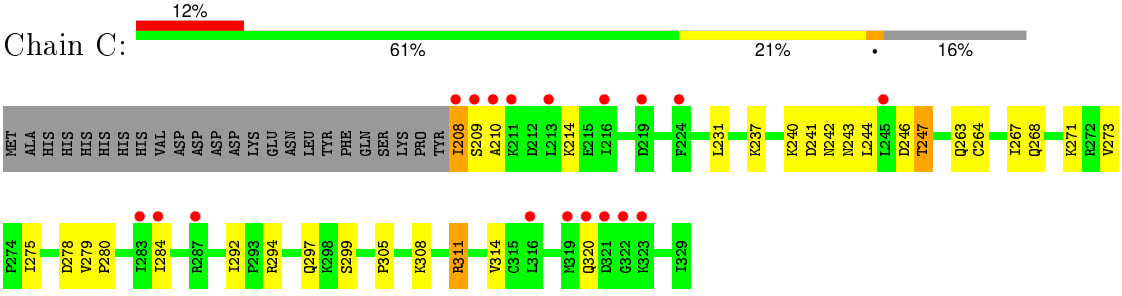
- Molecule 1: Polymerase cofactor

Chain B:



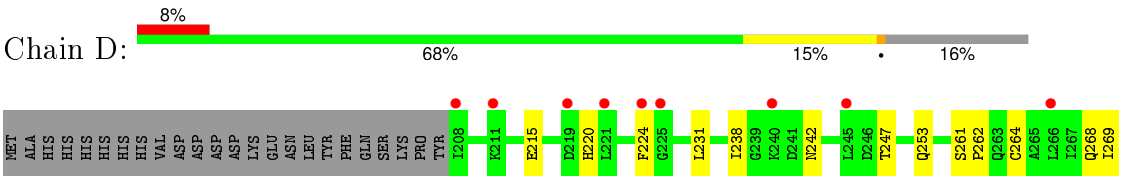
- Molecule 1: Polymerase cofactor

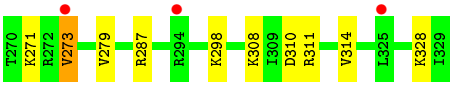
Chain C:



- Molecule 1: Polymerase cofactor

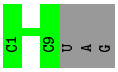
Chain D:





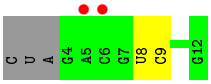
• Molecule 2: dsRNA

Chain E:



• Molecule 2: dsRNA

Chain F:

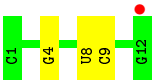


• Molecule 2: dsRNA

Chain J:

• Molecule 2: dsRNA

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.09Å 72.87Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.70 39.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.30-2.70) 99.5 (39.30-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.209 , 0.262 0.225 , 0.272	Depositor DCC
R_{free} test set	1016 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 20036 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4703	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.40	0/974	0.59	0/1317
1	B	0.39	0/974	0.60	0/1317
1	C	0.37	0/974	0.57	0/1317
1	D	0.38	0/974	0.59	0/1317
2	E	0.33	0/208	0.78	0/322
2	F	0.46	0/215	0.79	0/333
2	I	0.39	0/281	0.85	0/436
2	J	0.40	0/284	0.90	0/440
All	All	0.39	0/4884	0.65	0/6799

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	952	0	984	18	0
1	B	952	0	984	18	0
1	C	952	0	984	19	0
1	D	952	0	984	8	0
2	E	187	0	99	0	0
2	F	193	0	98	1	0
2	I	252	0	131	2	0
2	J	255	0	130	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	5	0	0	0	0
3	C	1	0	0	0	0
3	J	1	0	0	0	0
All	All	4703	0	4394	65	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 (65) 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:308:LYS:HB2	1:B:311:ARG:HG3	1.67	0.77
1:B:318:LYS:NZ	1:B:322:GLY:O	2.22	0.69
1:D:231:LEU:HD12	1:D:314:VAL:HG22	1.74	0.68
1:B:242:ASN:HD21	1:B:275:ILE:HG12	1.61	0.66
1:C:308:LYS:HB2	1:C:311:ARG:HG3	1.79	0.65
1:C:294:ARG:HA	1:C:297:GLN:HG2	1.80	0.64
1:B:238:ILE:HD13	1:B:279:VAL:HG21	1.82	0.61
1:C:292:ILE:O	1:C:297:GLN:NE2	2.32	0.61
1:C:264:CYS:O	1:C:268:GLN:HG2	2.02	0.59
1:B:287:ARG:HG2	1:B:291:ASP:OD2	2.02	0.58
1:A:275:ILE:O	1:A:275:ILE:HG13	2.04	0.57
1:B:275:ILE:O	1:B:279:VAL:HG22	2.04	0.57
1:A:319:MET:HG3	1:A:323:LYS:HB3	1.87	0.56
1:D:311:ARG:O	1:D:328:LYS:NZ	2.34	0.56
1:B:273:VAL:HG12	1:B:275:ILE:HG22	1.87	0.56
1:A:244:LEU:HD13	1:A:275:ILE:HG21	1.88	0.56
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.87	0.56
1:D:238:ILE:HD13	1:D:279:VAL:HG21	1.88	0.56
1:C:237:LYS:HE3	1:C:241:ASP:OD2	2.06	0.55
1:A:238:ILE:HD13	1:A:279:VAL:HG21	1.88	0.55
2:I:8:U:H2'	2:I:9:C:C6	2.42	0.55
1:A:289:ARG:HB2	1:A:319:MET:HE1	1.89	0.55
1:A:298:LYS:HE2	1:C:279:VAL:HG22	1.90	0.54
2:J:6:C:H2'	2:J:7:G:C8	2.44	0.53
1:A:289:ARG:N	1:A:319:MET:HE1	2.24	0.53
1:D:264:CYS:O	1:D:268:GLN:HG2	2.09	0.52
2:J:6:C:H2'	2:J:7:G:H8	1.74	0.52
1:B:279:VAL:HG12	1:C:305:PRO:HG3	1.90	0.52
1:A:264:CYS:O	1:A:268:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:HG12	1:C:305:PRO:CG	2.40	0.52
1:C:210:ALA:HB2	1:C:240:LYS:HD2	1.92	0.52
1:A:297:GLN:HG3	1:C:278:ASP:OD2	2.10	0.52
1:C:267:ILE:HG22	1:C:271:LYS:HD2	1.93	0.50
2:J:5:A:O2'	2:J:6:C:OP1	2.26	0.50
1:B:242:ASN:HD21	1:B:275:ILE:CG1	2.23	0.50
1:B:321:ASP:OD1	1:B:323:LYS:HB3	2.12	0.50
1:C:273:VAL:HG12	1:C:275:ILE:HG22	1.94	0.49
1:A:231:LEU:HD13	1:A:314:VAL:HG22	1.95	0.48
1:B:279:VAL:HG23	1:B:309:ILE:HD12	1.97	0.46
1:A:289:ARG:CA	1:A:319:MET:HE1	2.46	0.46
1:D:269:ILE:O	1:D:273:VAL:HG13	2.16	0.46
1:D:308:LYS:HD2	1:D:308:LYS:HA	1.67	0.45
1:B:308:LYS:HE3	1:B:310:ASP:OD1	2.16	0.45
1:B:262:PRO:O	1:B:266:LEU:HG	2.17	0.44
1:A:304:PRO:HD3	1:A:313:TRP:CZ2	2.52	0.44
1:B:244:LEU:HD12	1:B:275:ILE:CG2	2.47	0.44
1:C:214:LYS:HE2	1:C:214:LYS:HB3	1.63	0.44
1:A:266:LEU:O	1:A:269:ILE:HB	2.17	0.44
1:C:279:VAL:HG12	1:C:280:PRO:O	2.18	0.43
1:C:231:LEU:HD13	1:C:314:VAL:HG22	2.00	0.43
2:I:8:U:H2'	2:I:9:C:H6	1.83	0.43
1:A:225:GLY:O	1:A:295:ALA:HB3	2.19	0.43
1:C:263:GLN:O	1:C:267:ILE:HG13	2.19	0.42
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.60	0.42
1:A:313:TRP:CZ3	1:A:328:LYS:HB2	2.55	0.42
2:F:8:U:H2'	2:F:9:C:C6	2.55	0.42
1:D:271:LYS:HE2	1:D:310:ASP:O	2.20	0.41
1:B:242:ASN:HD21	1:B:275:ILE:CD1	2.33	0.41
1:B:279:VAL:HA	1:B:280:PRO:HD3	1.82	0.41
1:A:304:PRO:O	1:A:307:PRO:HD3	2.20	0.41
1:C:208:ILE:HG13	1:C:209:SER:N	2.35	0.41
1:C:244:LEU:HD22	1:C:247:THR:HB	2.02	0.40
1:D:220:HIS:HB3	1:D:262:PRO:HB3	2.03	0.40
1:A:279:VAL:HA	1:A:280:PRO:HD3	1.94	0.40
1:B:242:ASN:N	1:B:242:ASN:OD1	2.55	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	120/146 (82%)	120 (100%)	0	0	100	100
1	B	120/146 (82%)	119 (99%)	1 (1%)	0	100	100
1	C	120/146 (82%)	119 (99%)	1 (1%)	0	100	100
1	D	120/146 (82%)	120 (100%)	0	0	100	100
All	All	480/584 (82%)	478 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	106/129 (82%)	99 (93%)	7 (7%)	21	45
1	B	106/129 (82%)	100 (94%)	6 (6%)	25	53
1	C	106/129 (82%)	97 (92%)	9 (8%)	13	30
1	D	106/129 (82%)	97 (92%)	9 (8%)	13	30
All	All	424/516 (82%)	393 (93%)	31 (7%)	17	39

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	214	LYS

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Mol	Chain	Res	Type
1	A	242	ASN
1	A	275	ILE
1	A	288	SER
1	A	299	SER
1	A	319	MET
1	B	208	ILE
1	B	211	LYS
1	B	251	GLU
1	B	311	ARG
1	B	318	LYS
1	B	328	LYS
1	C	208	ILE
1	C	242	ASN
1	C	243	ASN
1	C	246	ASP
1	C	247	THR
1	C	284	ILE
1	C	299	SER
1	C	311	ARG
1	C	320	GLN
1	D	215	GLU
1	D	224	PHE
1	D	242	ASN
1	D	247	THR
1	D	253	GLN
1	D	261	SER
1	D	273	VAL
1	D	287	ARG
1	D	298	LYS

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

Mol	Chain	Res	Type
1	B	249	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	8/12 (66%)	0	0
2	F	8/12 (66%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	11/12 (91%)	1 (9%)	0
2	J	11/12 (91%)	3 (27%)	1 (9%)
All	All	38/48 (79%)	4 (10%)	1 (2%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	J	4	G
2	J	5	A
2	J	6	C
2	I	4	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	J	5	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, 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	122/146 (83%)	0.30	1 (0%) 87 88	18, 29, 45, 53	0
1	B	122/146 (83%)	0.31	0 100 100	16, 33, 54, 63	0
1	C	122/146 (83%)	0.89	18 (14%) 3 2	33, 50, 66, 77	0
1	D	122/146 (83%)	0.63	12 (9%) 10 7	31, 51, 64, 68	0
2	E	9/12 (75%)	0.53	0 100 100	27, 30, 76, 82	0
2	F	9/12 (75%)	0.66	2 (22%) 1 1	17, 44, 94, 96	0
2	I	12/12 (100%)	0.42	1 (8%) 14 11	45, 51, 83, 84	0
2	J	12/12 (100%)	1.82	5 (41%) 0 0	37, 65, 98, 100	0
All	All	530/632 (83%)	0.56	39 (7%) 17 15	16, 44, 66, 100	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	ASP	6.4
1	D	224	PHE	5.8
1	C	224	PHE	4.5
1	C	284	ILE	4.5
2	J	1	C	4.5
1	C	320	GLN	4.4
2	J	4	G	4.3
1	C	216	ILE	4.3
1	C	211	LYS	4.1
1	C	323	LYS	3.8
2	J	2	U	3.6
1	C	213	LEU	3.5
1	D	211	LYS	3.4
1	D	208	ILE	3.1
1	C	287	ARG	2.9
1	C	321	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	283	ILE	2.7
1	A	243	ASN	2.6
2	F	6	C	2.6
2	I	12	G	2.6
1	C	319	MET	2.6
1	C	316	LEU	2.6
2	F	5	A	2.6
1	C	208	ILE	2.4
1	D	266	LEU	2.4
1	D	245	LEU	2.3
2	J	5	A	2.3
1	C	322	GLY	2.3
1	C	210	ALA	2.3
1	D	225	GLY	2.3
1	D	221	LEU	2.3
1	C	209	SER	2.3
2	J	3	A	2.2
1	C	219	ASP	2.2
1	C	245	LEU	2.2
1	D	273	VAL	2.2
1	D	240	LYS	2.1
1	D	294	ARG	2.1
1	D	325	LEU	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.