Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 09:34 PM EST

PDB ID	:	4K4Z
Title	:	Coxsackievirus B3 polymerase elongation complex (r2_Mg_form)
Authors	:	Gong, P.; Peersen, O.B.
Deposited on	:	2013-04-12
Resolution	:	2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

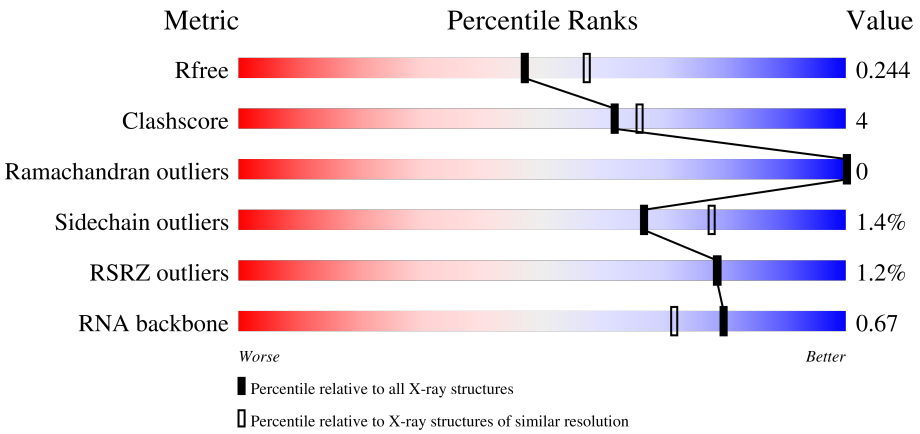
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)
RNA backbone	3102	1052 (2.60-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	472	2% 91% 7% •
1	E	472	% 86% 12% •
1	I	472	% 88% 10% •
1	M	472	2% 90% 8% • •

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Mol	Chain	Length	Quality of chain
2	B	24	29% 29% 12% 29%
2	F	24	29% 29% 8% 8% 25%
2	J	24	29% 33% 12% 25%
2	N	24	33% 12% 25% 29%
3	C	14	71% 21% 7%
3	G	14	71% 21% 7%
3	K	14	71% 21% 7%
3	O	14	79% 7% 7% 7%
4	D	9	22% 78%
4	H	9	44% 56%
4	L	9	11% 22% 67%
4	P	9	22% 11% 67%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18903 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3689	2370	613	684	22	0	0	0
1	E	462	3689	2370	613	684	22	0	0	0
1	I	462	3689	2370	613	684	22	0	0	0
1	M	462	3689	2370	613	684	22	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ILE	LEU	conflict	UNP Q66338
A	463	GLY	-	expression tag	UNP Q66338
A	464	SER	-	expression tag	UNP Q66338
A	465	SER	-	expression tag	UNP Q66338
A	466	SER	-	expression tag	UNP Q66338
A	467	HIS	-	expression tag	UNP Q66338
A	468	HIS	-	expression tag	UNP Q66338
A	469	HIS	-	expression tag	UNP Q66338
A	470	HIS	-	expression tag	UNP Q66338
A	471	HIS	-	expression tag	UNP Q66338
A	472	HIS	-	expression tag	UNP Q66338
E	252	ILE	LEU	conflict	UNP Q66338
E	463	GLY	-	expression tag	UNP Q66338
E	464	SER	-	expression tag	UNP Q66338
E	465	SER	-	expression tag	UNP Q66338
E	466	SER	-	expression tag	UNP Q66338
E	467	HIS	-	expression tag	UNP Q66338
E	468	HIS	-	expression tag	UNP Q66338
E	469	HIS	-	expression tag	UNP Q66338
E	470	HIS	-	expression tag	UNP Q66338
E	471	HIS	-	expression tag	UNP Q66338

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Chain	Residue	Modelled	Actual	Comment	Reference
E	472	HIS	-	expression tag	UNP Q66338
I	252	ILE	LEU	conflict	UNP Q66338
I	463	GLY	-	expression tag	UNP Q66338
I	464	SER	-	expression tag	UNP Q66338
I	465	SER	-	expression tag	UNP Q66338
I	466	SER	-	expression tag	UNP Q66338
I	467	HIS	-	expression tag	UNP Q66338
I	468	HIS	-	expression tag	UNP Q66338
I	469	HIS	-	expression tag	UNP Q66338
I	470	HIS	-	expression tag	UNP Q66338
I	471	HIS	-	expression tag	UNP Q66338
I	472	HIS	-	expression tag	UNP Q66338
M	252	ILE	LEU	conflict	UNP Q66338
M	463	GLY	-	expression tag	UNP Q66338
M	464	SER	-	expression tag	UNP Q66338
M	465	SER	-	expression tag	UNP Q66338
M	466	SER	-	expression tag	UNP Q66338
M	467	HIS	-	expression tag	UNP Q66338
M	468	HIS	-	expression tag	UNP Q66338
M	469	HIS	-	expression tag	UNP Q66338
M	470	HIS	-	expression tag	UNP Q66338
M	471	HIS	-	expression tag	UNP Q66338
M	472	HIS	-	expression tag	UNP Q66338

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	17	358	160	61	120	17	0	0	0
			Total	C	N	O	P			
2	F	18	378	169	63	128	18	0	0	0
			Total	C	N	O	P			
2	J	18	378	169	63	128	18	0	0	0
			Total	C	N	O	P			
2	N	17	358	160	61	120	17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	283	126	55	89	13	0	0	0
3	G	13	283	126	55	89	13	0	0	0
3	K	13	283	126	55	89	13	0	0	0
3	O	13	283	126	55	89	13	0	0	0

- Molecule 4 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	2	46	20	10	14	2	0	0	0
4	L	3	68	30	15	20	3	0	0	0
4	H	4	91	40	20	27	4	0	0	0
4	P	3	68	30	15	20	3	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	E	1	1	1	0	0
5	I	1	1	1	0	0
5	M	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	294	294	294	0	0
6	B	19	19	19	0	0
6	C	14	14	14	0	0

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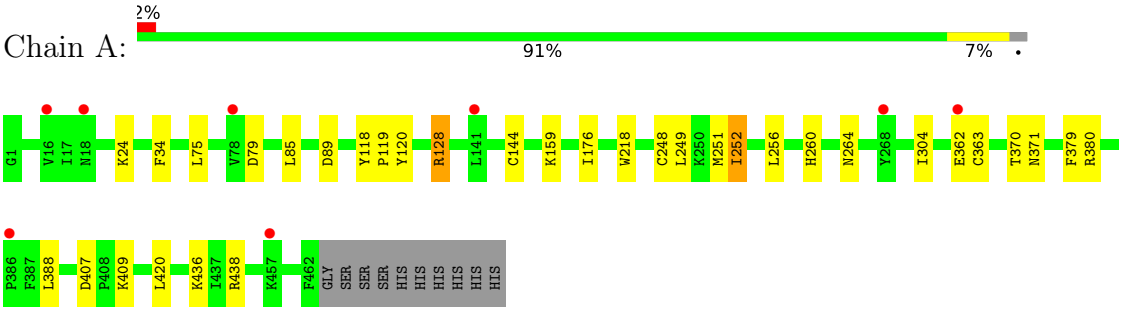
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	245	245	245	0	0
			Total	O		
6	F	20	20	20	0	0
			Total	O		
6	G	15	15	15	0	0
			Total	O		
6	I	281	281	281	0	0
			Total	O		
6	J	21	21	21	0	0
			Total	O		
6	K	19	19	19	0	0
			Total	O		
6	M	304	304	304	0	0
			Total	O		
6	N	21	21	21	0	0
			Total	O		
6	O	13	13	13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

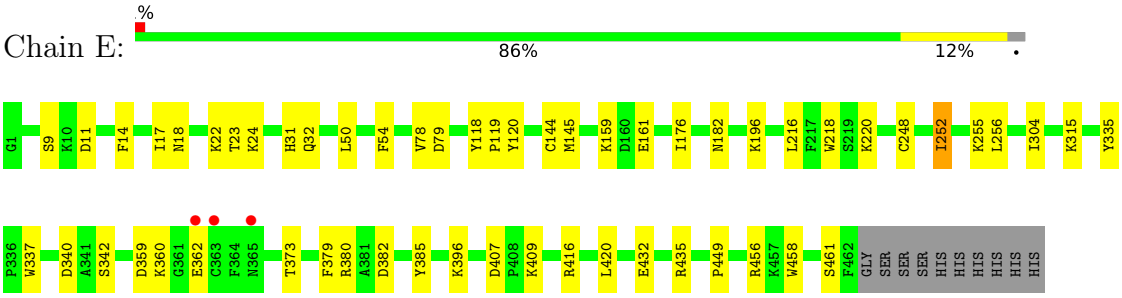
• Molecule 1: RNA-dependent RNA polymerase

Chain A:



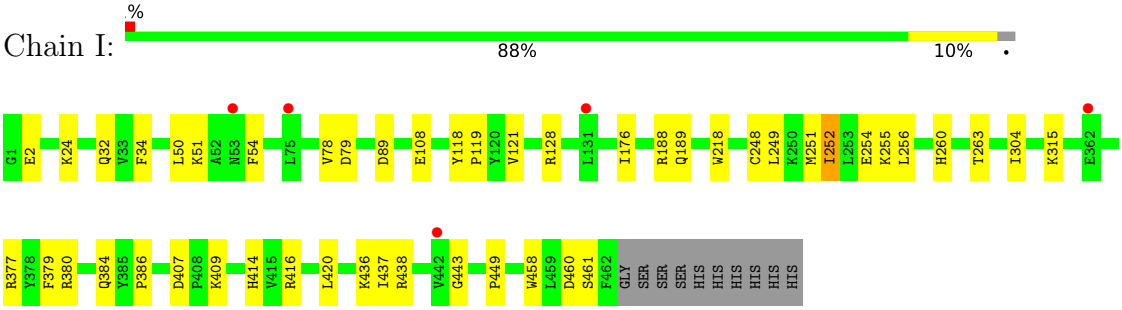
• Molecule 1: RNA-dependent RNA polymerase

Chain E:



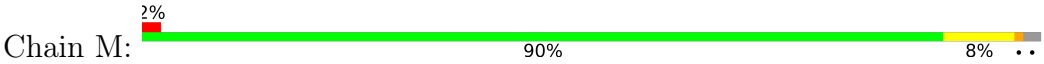
• Molecule 1: RNA-dependent RNA polymerase

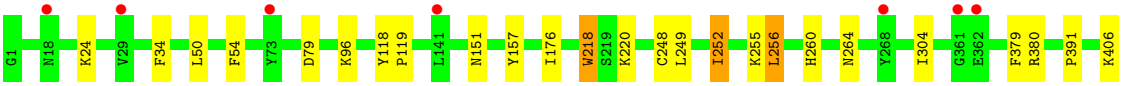
Chain I:



• Molecule 1: RNA-dependent RNA polymerase

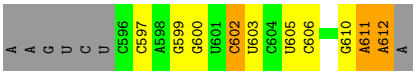
Chain M:





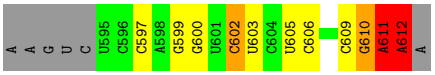
• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')

Chain B:



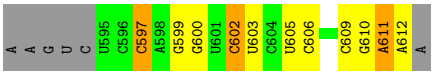
• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')

Chain F:



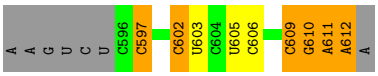
• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')

Chain J:



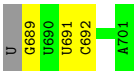
• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*GP*AP*AP*A)-3')

Chain N:



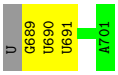
• Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain C:



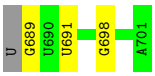
• Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain G:



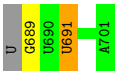
• Molecule 3: RNA (5'-R(*UP*GP*UP*UP*CP*GP*AP*CP*GP*AP*GP*AP*GP*A)-3')

Chain K:



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

Chain O:



• Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

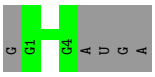
Chain D:

• Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain L:

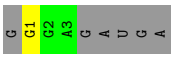
• Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain H:



• Molecule 4: RNA (5'-R(P*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.64Å 60.63Å 194.68Å 89.98° 89.92° 78.68°	Depositor
Resolution (Å)	45.58 – 2.17 45.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.58-2.17) 96.8 (45.58-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.204 , 0.244 0.205 , 0.244	Depositor DCC
R_{free} test set	8937 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.469 for -h,-k,l 0.446 for k,h,-l 0.446 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18903	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.45	0/3782	0.57	0/5120
1	E	0.44	0/3782	0.57	0/5120
1	I	0.44	0/3782	0.56	0/5120
1	M	0.46	0/3782	0.56	0/5120
2	B	0.59	0/398	1.02	0/617
2	F	0.63	0/420	1.11	2/651 (0.3%)
2	J	0.60	0/420	1.00	0/651
2	N	0.58	0/398	1.00	0/617
3	C	0.54	0/317	0.96	0/493
3	G	0.59	0/317	0.95	0/493
3	K	0.52	0/317	1.00	0/493
3	O	0.50	0/317	0.93	0/493
4	D	0.35	0/51	0.67	0/78
4	H	0.57	0/102	0.98	0/158
4	L	0.33	0/76	0.85	0/117
4	P	0.34	0/76	0.66	0/117
All	All	0.47	0/18337	0.67	2/25458 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	612	A	O5'-P-OP1	-7.85	98.63	105.70
2	F	611	A	O4'-C1'-N9	6.99	113.79	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3689	0	3658	22	0
1	E	3689	0	3658	33	0
1	I	3689	0	3658	33	0
1	M	3689	0	3658	25	0
2	B	358	0	184	9	0
2	F	378	0	194	12	0
2	J	378	0	194	7	0
2	N	358	0	184	9	0
3	C	283	0	142	4	0
3	G	283	0	142	3	0
3	K	283	0	142	3	0
3	O	283	0	142	2	0
4	D	46	0	23	0	0
4	H	91	0	45	0	0
4	L	68	0	34	1	0
4	P	68	0	34	1	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	294	0	0	6	0
6	B	19	0	0	0	0
6	C	14	0	0	0	0
6	E	245	0	0	6	0
6	F	20	0	0	0	0
6	G	15	0	0	0	0
6	I	281	0	0	11	0
6	J	21	0	0	0	0
6	K	19	0	0	0	0
6	M	304	0	0	8	0
6	N	21	0	0	1	0
6	O	13	0	0	0	0
All	All	18903	0	16092	144	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 4.

All (144) 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:M:96:LYS:NZ	6:M:835:HOH:O	2.08	0.87
1:A:264:ASN:OD1	6:A:812:HOH:O	1.98	0.80
3:C:689:G:N1	3:G:689:G:O6	2.15	0.79
1:E:360:LYS:NZ	6:E:759:HOH:O	2.15	0.79
2:B:610:G:H1	3:C:692:C:H42	1.29	0.78
1:A:388:LEU:O	6:A:748:HOH:O	2.05	0.73
1:A:379:PHE:O	1:A:380:ARG:NH1	2.21	0.71
3:C:689:G:H22	3:G:689:G:H1	1.37	0.71
1:E:315:LYS:NZ	6:E:649:HOH:O	2.22	0.70
1:I:379:PHE:O	1:I:380:ARG:NH1	2.24	0.70
2:N:609:C:C2'	2:N:610:G:H5'	2.22	0.69
2:F:612:A:H61	3:G:690:U:H3	1.38	0.69
2:N:610:G:H2'	2:N:611:A:C8	2.27	0.69
2:N:609:C:H2'	2:N:610:G:H5'	1.74	0.69
2:J:597:C:N4	4:L:1:G:O6	2.16	0.68
1:M:79:ASP:OD1	1:M:255:LYS:HE3	1.94	0.68
1:I:128:ARG:NH1	6:I:730:HOH:O	2.25	0.67
2:F:611:A:H1'	2:F:612:A:P	2.36	0.66
2:N:605:U:OP1	6:N:708:HOH:O	2.12	0.65
1:A:251:MET:SD	6:I:846:HOH:O	2.54	0.65
1:E:159:LYS:NZ	1:E:161:GLU:OE2	2.30	0.64
2:J:610:G:H2'	2:J:611:A:C8	2.32	0.64
1:M:264:ASN:OD1	6:M:836:HOH:O	2.14	0.64
1:M:379:PHE:O	1:M:380:ARG:NH1	2.31	0.64
1:E:379:PHE:O	1:E:380:ARG:NH1	2.30	0.64
2:F:611:A:O2'	2:F:612:A:OP1	2.12	0.64
2:F:602:C:H2'	2:F:603:U:C6	2.33	0.64
1:A:252:ILE:HG21	1:A:304:ILE:HD11	1.79	0.64
1:I:460:ASP:OD1	6:I:807:HOH:O	2.14	0.63
3:K:689:G:O4'	2:N:612:A:H2'	1.98	0.63
1:E:79:ASP:OD1	1:E:255:LYS:HE3	1.99	0.63
1:I:79:ASP:OD1	1:I:255:LYS:HE3	2.00	0.61
1:A:128:ARG:NH1	6:A:849:HOH:O	2.33	0.60
1:M:220:LYS:NZ	6:M:843:HOH:O	2.25	0.60
1:M:420:LEU:HD11	2:N:606:C:H4'	1.83	0.60
1:E:11:ASP:OD1	6:E:813:HOH:O	2.15	0.59
1:A:248:CYS:O	1:A:252:ILE:HG22	2.03	0.59
1:I:176:ILE:HD12	2:J:600:G:C8	2.38	0.59
1:E:176:ILE:HD12	2:F:600:G:C8	2.39	0.58
1:M:252:ILE:HG21	1:M:304:ILE:HD11	1.84	0.58
2:J:602:C:H2'	2:J:603:U:C6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ARG:NH2	6:E:693:HOH:O	2.28	0.56
1:E:24:LYS:HE3	2:F:599:G:O6	2.05	0.56
1:E:432:GLU:OE2	1:E:435:ARG:NH2	2.34	0.56
1:I:121:VAL:HG11	6:I:680:HOH:O	2.06	0.55
2:N:602:C:H2'	2:N:603:U:C6	2.41	0.55
1:A:420:LEU:HD21	2:B:606:C:H4'	1.88	0.55
2:B:610:G:H1	3:C:692:C:N4	2.01	0.55
1:A:362:GLU:OE1	1:A:362:GLU:N	2.33	0.55
2:B:602:C:H2'	2:B:603:U:C6	2.42	0.54
1:M:151:ASN:ND2	6:M:857:HOH:O	2.40	0.54
1:M:458:TRP:O	1:M:461:SER:OG	2.24	0.54
1:M:24:LYS:HE2	1:M:406:LYS:HD3	1.90	0.54
1:A:159:LYS:NZ	6:A:876:HOH:O	2.40	0.54
1:E:360:LYS:NZ	6:E:761:HOH:O	1.99	0.53
2:F:610:G:O2'	2:F:611:A:H5'	2.09	0.53
1:M:248:CYS:O	1:M:252:ILE:HG22	2.09	0.53
2:B:605:U:H2'	2:B:606:C:C6	2.43	0.52
1:M:444:ARG:NH2	6:M:685:HOH:O	2.36	0.52
1:A:371:ASN:O	6:A:796:HOH:O	2.19	0.52
2:B:611:A:O2'	2:B:612:A:O5'	2.25	0.52
1:A:176:ILE:HD12	2:B:600:G:C8	2.45	0.52
1:M:416:ARG:NH1	6:M:619:HOH:O	2.43	0.52
1:A:249:LEU:O	1:A:252:ILE:HG23	2.10	0.52
2:N:597:C:H42	4:P:1:G:H1	1.58	0.52
1:M:157:TYR:HB2	1:M:176:ILE:HD11	1.92	0.52
2:F:605:U:H2'	2:F:606:C:C6	2.44	0.51
1:I:377:ARG:NH1	6:I:629:HOH:O	2.39	0.51
2:J:605:U:H2'	2:J:606:C:C6	2.46	0.51
1:I:2:GLU:OE1	6:I:654:HOH:O	2.20	0.51
1:E:420:LEU:HD11	2:F:606:C:H4'	1.92	0.50
1:I:252:ILE:HG21	1:I:304:ILE:HD11	1.92	0.50
3:O:691:U:OP1	3:O:691:U:H4'	2.10	0.50
1:M:457:LYS:O	6:M:860:HOH:O	2.19	0.50
1:A:407:ASP:OD2	1:A:409:LYS:HE3	2.11	0.50
1:E:340:ASP:OD1	1:E:342:SER:OG	2.28	0.49
1:E:17:ILE:O	1:E:18:ASN:HB3	2.13	0.49
1:I:254:GLU:HG3	1:I:263:THR:HG21	1.95	0.49
1:I:248:CYS:O	1:I:252:ILE:HG22	2.12	0.49
1:E:252:ILE:HG21	1:E:304:ILE:HD11	1.95	0.49
1:I:438:ARG:NH2	6:I:772:HOH:O	2.41	0.49
1:I:315:LYS:O	6:I:673:HOH:O	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:HG13	1:E:252:ILE:HB	1.96	0.48
1:I:24:LYS:HE3	2:J:599:G:O6	2.13	0.48
1:I:420:LEU:HD21	2:J:606:C:H4'	1.95	0.48
1:I:409:LYS:NZ	6:I:702:HOH:O	2.39	0.48
1:I:437:ILE:O	1:I:443:GLY:HA3	2.13	0.48
2:F:602:C:H2'	2:F:603:U:H6	1.78	0.47
1:I:416:ARG:NH1	6:I:750:HOH:O	2.48	0.47
1:E:362:GLU:OE1	1:E:362:GLU:N	2.42	0.47
1:A:370:THR:O	1:A:380:ARG:NH2	2.41	0.46
1:E:248:CYS:O	1:E:252:ILE:HG22	2.15	0.46
1:A:85:LEU:HD12	1:A:252:ILE:HD11	1.98	0.46
1:I:416:ARG:HH12	1:I:449:PRO:HB3	1.80	0.46
1:I:458:TRP:O	1:I:461:SER:OG	2.24	0.46
1:M:256:LEU:HD12	1:M:256:LEU:HA	1.84	0.45
1:E:458:TRP:O	1:E:461:SER:OG	2.27	0.45
1:I:407:ASP:OD2	1:I:409:LYS:HE3	2.16	0.45
1:E:407:ASP:OD2	1:E:409:LYS:HE3	2.17	0.45
2:F:610:G:H4'	2:F:611:A:OP1	2.17	0.44
1:I:108:GLU:O	1:I:188:ARG:NH2	2.32	0.44
1:I:118:TYR:CG	1:I:119:PRO:HA	2.52	0.44
1:I:78:VAL:HG13	1:I:252:ILE:HB	1.99	0.44
1:A:118:TYR:CG	1:A:119:PRO:HA	2.53	0.44
1:E:118:TYR:CG	1:E:119:PRO:HA	2.52	0.44
1:M:50:LEU:HD11	1:M:54:PHE:HB2	1.99	0.44
1:E:220:LYS:NZ	6:E:838:HOH:O	2.34	0.44
2:N:605:U:H2'	2:N:606:C:C6	2.53	0.43
1:M:34:PHE:CE2	1:M:436:LYS:HE3	2.54	0.43
1:E:335:TYR:CE2	1:E:337:TRP:HE3	2.37	0.43
1:M:118:TYR:CG	1:M:119:PRO:HA	2.53	0.43
1:M:249:LEU:O	1:M:252:ILE:HG23	2.18	0.43
1:E:145:MET:HA	1:E:182:ASN:ND2	2.34	0.42
1:A:24:LYS:HE3	2:B:599:G:O6	2.20	0.42
1:M:423:TRP:CH2	1:M:455:ARG:HA	2.54	0.42
1:A:120:TYR:OH	1:A:144:CYS:HB3	2.19	0.42
1:E:9:SER:HB3	1:E:14:PHE:HB2	2.01	0.42
1:I:384:GLN:O	1:I:386:PRO:HD3	2.20	0.42
1:A:34:PHE:CE1	1:A:436:LYS:HE3	2.55	0.42
3:K:689:G:H22	3:O:689:G:H1	1.68	0.42
2:B:611:A:HO2'	2:B:612:A:C5'	2.32	0.42
1:E:416:ARG:HH12	1:E:449:PRO:HB3	1.85	0.42
6:A:768:HOH:O	1:I:251:MET:SD	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:249:LEU:O	1:I:252:ILE:HG23	2.20	0.41
1:E:382:ASP:HB3	1:E:385:TYR:O	2.19	0.41
1:I:189:GLN:NE2	6:I:693:HOH:O	2.34	0.41
1:E:22:LYS:HD2	1:E:23:THR:H	1.84	0.41
1:I:50:LEU:O	1:I:51:LYS:HD3	2.20	0.41
1:I:414:HIS:CD2	3:K:698:G:H4'	2.56	0.41
1:I:50:LEU:HD11	1:I:54:PHE:HB2	2.02	0.41
1:E:50:LEU:HD11	1:E:54:PHE:HB2	2.02	0.41
1:E:120:TYR:OH	1:E:144:CYS:HB3	2.21	0.41
1:M:218:TRP:CD1	1:M:391:PRO:HA	2.56	0.41
1:M:432:GLU:OE2	1:M:435:ARG:NH2	2.47	0.41
1:A:75:LEU:HD22	1:A:251:MET:HE1	2.03	0.40
1:A:362:GLU:HG2	1:A:363:CYS:N	2.36	0.40
1:E:31:HIS:HD2	1:E:32:GLN:NE2	2.19	0.40
2:F:610:G:H3'	2:F:611:A:C8	2.56	0.40
1:I:118:TYR:CD1	1:I:119:PRO:HA	2.56	0.40
1:M:462:PHE:O	6:M:875:HOH:O	2.21	0.40
1:E:359:ASP:OD1	1:E:373:THR:OG1	2.35	0.40
1:I:34:PHE:CE2	1:I:436:LYS:HE3	2.56	0.40
1:M:407:ASP:HA	1:M:408:PRO:HD2	1.89	0.40
1:E:396:LYS:HE3	1:E:396:LYS:HB2	1.91	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	460/472 (98%)	454 (99%)	6 (1%)	0	100	100
1	E	460/472 (98%)	453 (98%)	7 (2%)	0	100	100
1	I	460/472 (98%)	455 (99%)	5 (1%)	0	100	100
1	M	460/472 (98%)	455 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1840/1888 (98%)	1817 (99%)	23 (1%)	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	404/413 (98%)	396 (98%)	8 (2%)	55	66
1	E	404/413 (98%)	399 (99%)	5 (1%)	71	81
1	I	404/413 (98%)	398 (98%)	6 (2%)	65	76
1	M	404/413 (98%)	400 (99%)	4 (1%)	76	85
All	All	1616/1652 (98%)	1593 (99%)	23 (1%)	67	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	89	ASP
1	A	128	ARG
1	A	218	TRP
1	A	252	ILE
1	A	256	LEU
1	A	260	HIS
1	A	438	ARG
1	E	196	LYS
1	E	216	LEU
1	E	218	TRP
1	E	252	ILE
1	E	256	LEU
1	I	32	GLN
1	I	89	ASP
1	I	218	TRP
1	I	252	ILE

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Mol	Chain	Res	Type
1	I	256	LEU
1	I	260	HIS
1	M	218	TRP
1	M	252	ILE
1	M	256	LEU
1	M	260	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	HIS
1	E	32	GLN
1	M	32	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/24 (66%)	4 (25%)	1 (6%)
2	F	17/24 (70%)	6 (35%)	2 (11%)
2	J	17/24 (70%)	5 (29%)	1 (5%)
2	N	16/24 (66%)	6 (37%)	0
3	C	12/14 (85%)	1 (8%)	0
3	G	12/14 (85%)	1 (8%)	0
3	K	12/14 (85%)	1 (8%)	0
3	O	12/14 (85%)	1 (8%)	0
4	D	1/9 (11%)	0	0
4	H	3/9 (33%)	0	0
4	L	2/9 (22%)	1 (50%)	0
4	P	2/9 (22%)	0	0
All	All	122/188 (64%)	26 (21%)	4 (3%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	597	C
2	B	602	C
2	B	611	A
2	B	612	A
3	C	691	U
2	F	597	C

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Mol	Chain	Res	Type
2	F	602	C
2	F	609	C
2	F	610	G
2	F	611	A
2	F	612	A
3	G	691	U
2	J	597	C
2	J	602	C
2	J	609	C
2	J	611	A
2	J	612	A
3	K	691	U
4	L	3	A
2	N	597	C
2	N	602	C
2	N	609	C
2	N	610	G
2	N	611	A
2	N	612	A
3	O	691	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	611	A
2	F	610	G
2	F	611	A
2	J	611	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	462/472 (97%)	0.09	8 (1%)	70	70	22, 34, 50, 83	0
1	E	462/472 (97%)	0.09	3 (0%)	89	89	22, 34, 48, 79	0
1	I	462/472 (97%)	0.07	5 (1%)	80	80	21, 35, 49, 77	0
1	M	462/472 (97%)	0.15	8 (1%)	70	70	22, 35, 49, 73	0
2	B	17/24 (70%)	-0.42	0	100	100	30, 43, 99, 105	0
2	F	18/24 (75%)	-0.34	0	100	100	30, 50, 105, 111	0
2	J	18/24 (75%)	-0.45	0	100	100	30, 51, 105, 113	0
2	N	17/24 (70%)	-0.45	0	100	100	30, 45, 98, 103	0
3	C	13/14 (92%)	-0.40	0	100	100	26, 53, 104, 105	0
3	G	13/14 (92%)	-0.33	0	100	100	27, 52, 104, 108	0
3	K	13/14 (92%)	-0.34	0	100	100	27, 53, 104, 105	0
3	O	13/14 (92%)	-0.41	0	100	100	27, 54, 106, 108	0
4	D	2/9 (22%)	0.69	0	100	100	84, 84, 84, 88	0
4	H	4/9 (44%)	0.55	0	100	100	60, 95, 106, 111	0
4	L	3/9 (33%)	0.53	0	100	100	92, 92, 94, 99	0
4	P	3/9 (33%)	0.52	0	100	100	85, 85, 86, 95	0
All	All	1982/2076 (95%)	0.07	24 (1%)	79	79	21, 35, 55, 113	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	4.1
1	M	18	ASN	3.5
1	A	18	ASN	3.5
1	M	361	GLY	3.4
1	A	362	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	141	LEU	3.1
1	M	362	GLU	2.9
1	A	268	TYR	2.8
1	I	362	GLU	2.6
1	M	29	VAL	2.5
1	E	365	ASN	2.5
1	I	53	ASN	2.5
1	A	78	VAL	2.4
1	M	268	TYR	2.4
1	I	131	LEU	2.3
1	E	363	CYS	2.2
1	E	362	GLU	2.2
1	A	457	LYS	2.1
1	M	73	TYR	2.1
1	A	16	VAL	2.1
1	I	442	VAL	2.1
1	I	75	LEU	2.0
1	M	462	PHE	2.0
1	A	386	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
5	MG	M	501	1/1	0.79	0.05	40,40,40,40	0
5	MG	A	501	1/1	0.84	0.04	40,40,40,40	0
5	MG	E	501	1/1	0.94	0.04	36,36,36,36	0
5	MG	I	501	1/1	0.98	0.05	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.