Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:08 AM GMT

PDB ID	:	1ZR4
Title	:	Structure of a Synaptic gamma-delta Resolvase Tetramer Covalently linked to two Cleaved DNAs
Authors	:	Li, W.; Kamtekar, S.; Xiong, Y.; Sarkis, G.J.; Grindley, N.D.; Steitz, T.A.
Deposited on	:	2005-05-19
Resolution	:	3.40 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:

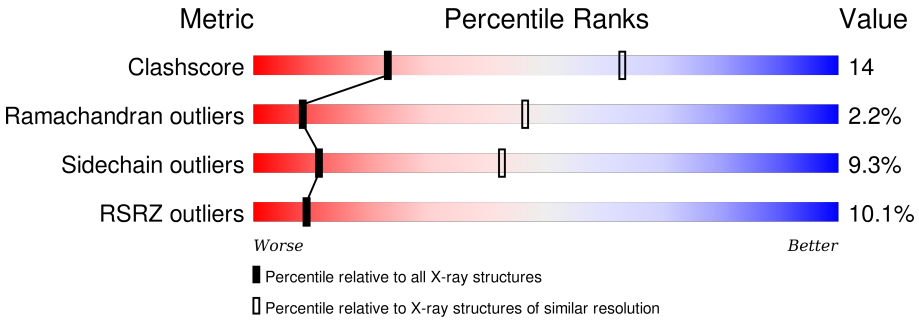
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	J	19	32% 53% 42% 5%
1	M	19	11% 26% 37% 37%
1	U	19	11% 32% 37% 32%
1	X	19	5% 21% 42% 37%
2	I	3	67% 33%
2	O	3	67% 33%
2	W	3	67% 33%

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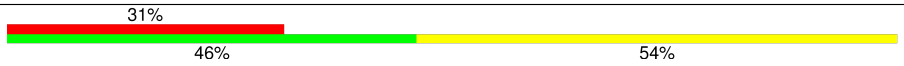
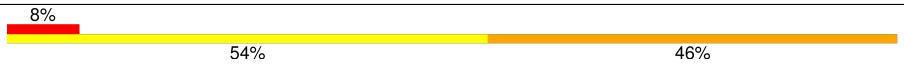
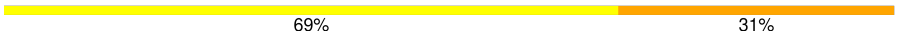
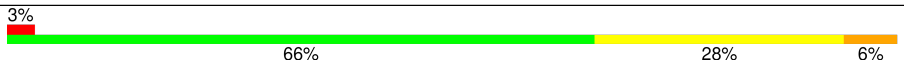
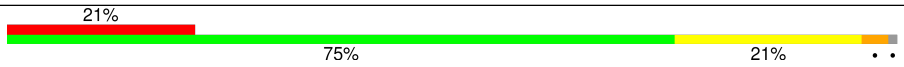
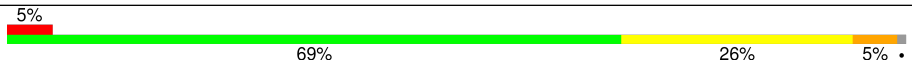
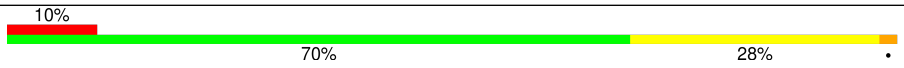
Mol	Chain	Length	Quality of chain
2	Z	3	
3	K	13	
3	N	13	
3	V	13	
3	Y	13	
4	A	183	
4	B	183	
4	D	183	
4	E	183	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8516 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 DNA chain called TCAGTGTCCGATAATTTAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	19	Total	C	N	O	P	0	0	0
			385	187	65	115	18			
1	J	19	Total	C	N	O	P	0	0	0
			385	187	65	115	18			
1	U	19	Total	C	N	O	P	0	0	0
			385	187	65	115	18			
1	M	19	Total	C	N	O	P	0	0	0
			385	187	65	115	18			

- Molecule 2 is a DNA chain called AAA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	3	Total	C	N	O	P	0	0	0
			63	30	15	15	3			
2	I	3	Total	C	N	O	P	0	0	0
			63	30	15	15	3			
2	W	3	Total	C	N	O	P	0	0	0
			63	30	15	15	3			
2	O	3	Total	C	N	O	P	0	0	0
			63	30	15	15	3			

- Molecule 3 is a DNA chain called TTATCGGACACTG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	13	Total	C	N	O	P	0	0	0
			263	127	47	77	12			
3	K	13	Total	C	N	O	P	0	0	0
			263	127	47	77	12			
3	V	13	Total	C	N	O	P	0	0	0
			263	127	47	77	12			
3	N	13	Total	C	N	O	P	0	0	0
			263	127	47	77	12			

- Molecule 4 is a protein called Transposon gamma-delta resolvase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	183	Total	C	N	O	S	0	0	0
			1422	881	266	268	7			
4	B	182	Total	C	N	O	S	0	0	0
			1414	876	265	267	6			
4	E	183	Total	C	N	O	S	0	0	0
			1422	881	266	268	7			
4	D	182	Total	C	N	O	S	0	0	0
			1414	876	265	267	6			

There are 24 discrepancies between the modelled and reference sequences:

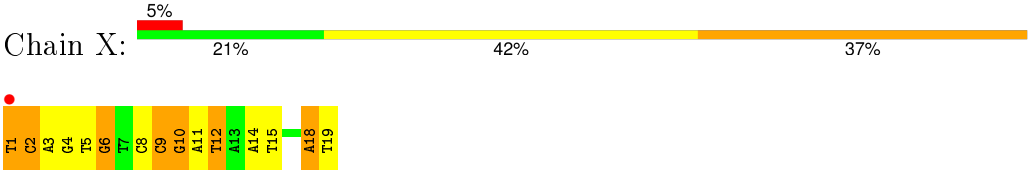
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	ARG	ENGINEERED	UNP P03012
A	56	LYS	GLU	ENGINEERED	UNP P03012
A	101	SER	GLY	ENGINEERED	UNP P03012
A	102	TYR	GLU	ENGINEERED	UNP P03012
A	103	ILE	MET	ENGINEERED	UNP P03012
A	124	GLN	GLU	ENGINEERED	UNP P03012
B	2	ALA	ARG	ENGINEERED	UNP P03012
B	56	LYS	GLU	ENGINEERED	UNP P03012
B	101	SER	GLY	ENGINEERED	UNP P03012
B	102	TYR	GLU	ENGINEERED	UNP P03012
B	103	ILE	MET	ENGINEERED	UNP P03012
B	124	GLN	GLU	ENGINEERED	UNP P03012
E	2	ALA	ARG	ENGINEERED	UNP P03012
E	56	LYS	GLU	ENGINEERED	UNP P03012
E	101	SER	GLY	ENGINEERED	UNP P03012
E	102	TYR	GLU	ENGINEERED	UNP P03012
E	103	ILE	MET	ENGINEERED	UNP P03012
E	124	GLN	GLU	ENGINEERED	UNP P03012
D	2	ALA	ARG	ENGINEERED	UNP P03012
D	56	LYS	GLU	ENGINEERED	UNP P03012
D	101	SER	GLY	ENGINEERED	UNP P03012
D	102	TYR	GLU	ENGINEERED	UNP P03012
D	103	ILE	MET	ENGINEERED	UNP P03012
D	124	GLN	GLU	ENGINEERED	UNP P03012

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.

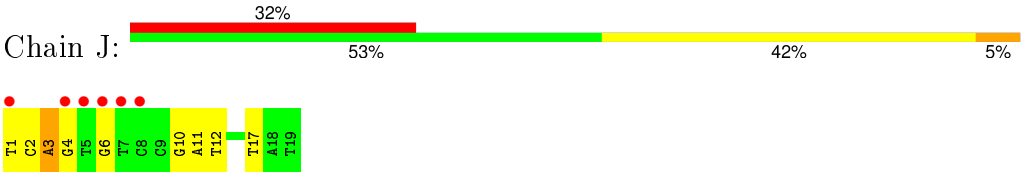
- Molecule 1: TCAGTGTCCGATAATTTAT

Chain X:



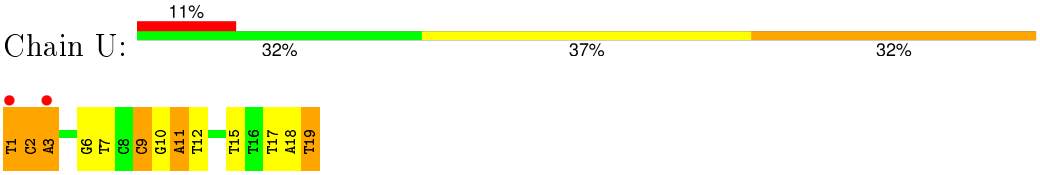
- Molecule 1: TCAGTGTCCGATAATTTAT

Chain J:



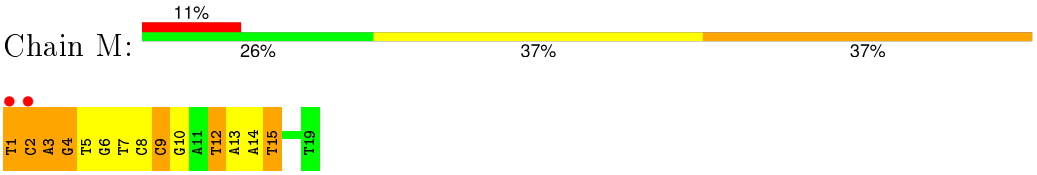
- Molecule 1: TCAGTGTCCGATAATTTAT

Chain U:



- Molecule 1: TCAGTGTCCGATAATTTAT

Chain M:



- Molecule 2: AAA

Chain Z:

- Molecule 2: AAA

Chain I:

• Molecule 2: AAA

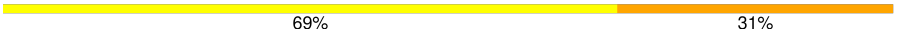
Chain W:

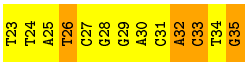
• Molecule 2: AAA

Chain O:

• Molecule 3: TTATCGGACACTG

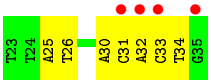
Chain Y:





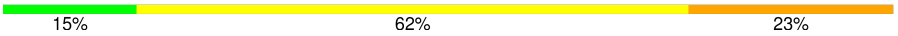
• Molecule 3: TTATCGGACACTG

Chain K:



• Molecule 3: TTATCGGACACTG

Chain V:

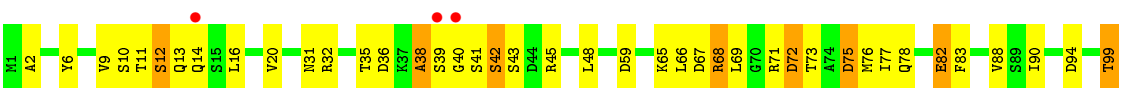


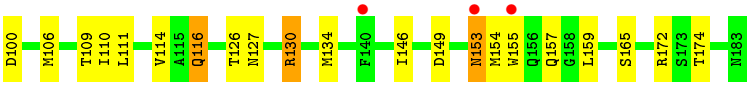
• Molecule 3: TTATCGGACACTG

Chain N:

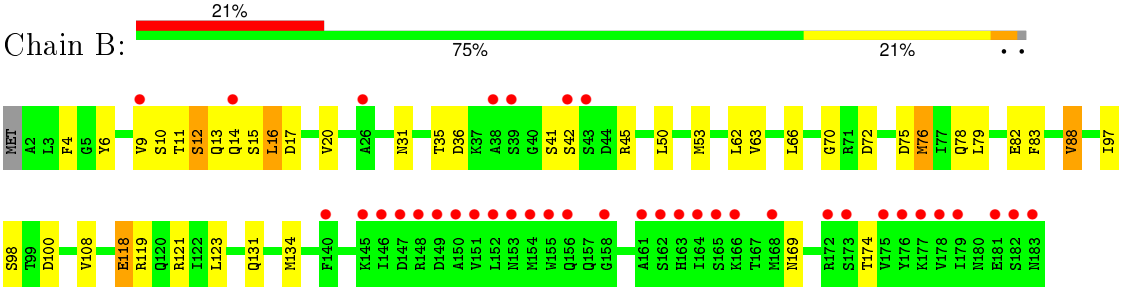
• Molecule 4: Transposon gamma-delta resolvase

Chain A:

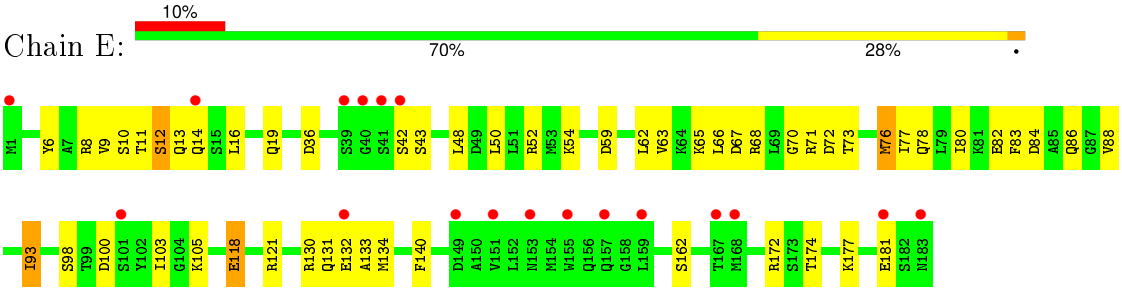




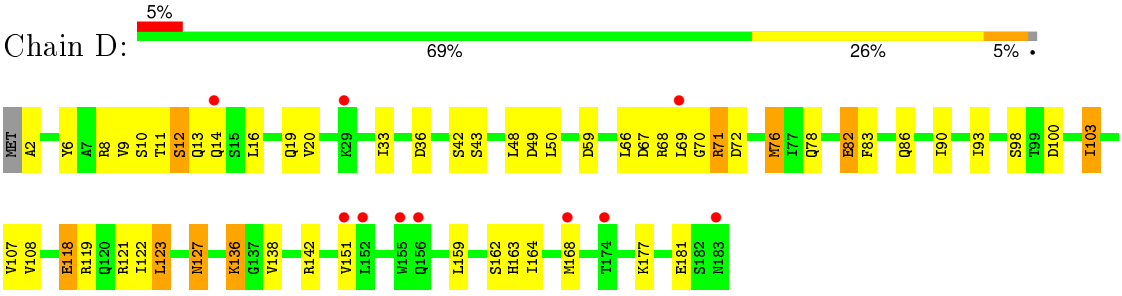
• Molecule 4: Transposon gamma-delta resolvase



• Molecule 4: Transposon gamma-delta resolvase



• Molecule 4: Transposon gamma-delta resolvase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.16Å 127.29Å 140.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 43.57 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.40) 99.4 (43.57-3.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.264 , 0.295 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	82.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33091 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8516	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	J	0.78	0/430	1.43	5/662 (0.8%)
1	M	1.06	1/430 (0.2%)	1.82	12/662 (1.8%)
1	U	0.83	0/430	1.64	10/662 (1.5%)
1	X	0.93	0/430	2.01	15/662 (2.3%)
2	I	0.53	0/71	1.09	0/107
2	O	0.90	0/71	1.25	0/107
2	W	0.64	0/71	1.13	0/107
2	Z	0.68	0/71	1.02	0/107
3	K	0.69	0/294	1.28	0/452
3	N	1.04	1/294 (0.3%)	1.91	11/452 (2.4%)
3	V	0.68	0/294	1.53	4/452 (0.9%)
3	Y	0.81	0/294	1.77	7/452 (1.5%)
4	A	0.49	0/1432	0.66	0/1914
4	B	0.46	0/1424	0.61	0/1904
4	D	0.46	0/1424	0.67	1/1902 (0.1%)
4	E	0.47	0/1432	0.61	0/1914
All	All	0.64	2/8892 (0.0%)	1.15	65/12518 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	34	DT	C1'-N1	5.96	1.56	1.49
1	M	1	DT	C1'-N1	5.10	1.55	1.49

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2	DC	O4'-C1'-N1	15.64	118.95	108.00
1	X	1	DT	O4'-C1'-N1	12.22	116.56	108.00
3	N	26	DT	C6-C5-C7	-9.86	116.99	122.90
3	Y	24	DT	C6-C5-C7	-9.82	117.01	122.90
1	X	1	DT	C1'-O4'-C4'	-9.01	101.09	110.10
1	M	3	DA	P-O3'-C3'	8.52	129.92	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	15	DT	O4'-C1'-N1	8.44	113.91	108.00
1	X	1	DT	C3'-C2'-C1'	-8.44	92.38	102.50
1	M	1	DT	O4'-C1'-N1	8.24	113.77	108.00
3	N	34	DT	O4'-C1'-N1	8.12	113.69	108.00
1	X	1	DT	P-O3'-C3'	8.05	129.36	119.70
1	X	2	DC	C1'-O4'-C4'	-7.94	102.16	110.10
1	M	7	DT	C6-C5-C7	-7.58	118.36	122.90
1	J	1	DT	P-O3'-C3'	7.57	128.78	119.70
3	Y	33	DC	O4'-C1'-N1	7.30	113.11	108.00
3	N	25	DA	O4'-C4'-C3'	-7.07	101.67	104.50
1	U	1	DT	O4'-C1'-N1	7.05	112.94	108.00
1	J	3	DA	P-O3'-C3'	6.98	128.08	119.70
3	Y	35	DG	C8-N9-C4	-6.83	103.67	106.40
1	M	1	DT	P-O3'-C3'	6.73	127.77	119.70
3	V	28	DG	O4'-C1'-N9	6.60	112.62	108.00
3	N	29	DG	O4'-C1'-N9	6.18	112.33	108.00
1	X	14	DA	C3'-C2'-C1'	-6.17	95.09	102.50
3	V	34	DT	C6-C5-C7	-6.12	119.23	122.90
3	N	24	DT	N3-C4-O4	6.07	123.54	119.90
1	X	9	DC	O4'-C1'-N1	5.93	112.15	108.00
3	N	23	DT	O4'-C1'-N1	5.90	112.13	108.00
1	M	9	DC	O4'-C1'-N1	5.85	112.09	108.00
3	Y	35	DG	N7-C8-N9	5.84	116.02	113.10
3	Y	32	DA	O4'-C1'-N9	5.80	112.06	108.00
1	M	14	DA	P-O3'-C3'	5.72	126.56	119.70
1	U	2	DC	N1-C2-O2	5.70	122.32	118.90
1	U	3	DA	P-O3'-C3'	5.63	126.45	119.70
1	U	12	DT	O4'-C1'-N1	5.60	111.92	108.00
1	U	11	DA	O4'-C1'-N9	5.58	111.91	108.00
3	V	24	DT	O4'-C1'-N1	5.57	111.90	108.00
1	U	2	DC	C1'-O4'-C4'	-5.54	104.56	110.10
4	D	138	VAL	N-CA-C	-5.53	96.07	111.00
1	J	17	DT	O4'-C1'-N1	5.52	111.86	108.00
1	U	7	DT	N3-C4-O4	5.50	123.20	119.90
1	X	12	DT	O4'-C1'-N1	5.50	111.85	108.00
3	Y	26	DT	C5-C4-O4	-5.50	121.05	124.90
1	M	2	DC	P-O3'-C3'	5.49	126.29	119.70
1	X	6	DG	P-O3'-C3'	5.45	126.24	119.70
3	N	27	DC	C4-C5-C6	5.44	120.12	117.40
1	X	18	DA	O4'-C1'-N9	5.43	111.80	108.00
1	M	12	DT	C1'-O4'-C4'	-5.41	104.69	110.10
1	X	1	DT	C5-C4-O4	-5.40	121.12	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	4	DG	O4'-C1'-N9	5.40	111.78	108.00
3	N	24	DT	C5-C4-O4	-5.40	121.12	124.90
3	N	28	DG	C1'-O4'-C4'	-5.34	104.76	110.10
3	V	33	DC	O4'-C1'-N1	5.32	111.72	108.00
1	X	10	DG	P-O3'-C3'	5.29	126.05	119.70
1	J	6	DG	P-O3'-C3'	5.28	126.04	119.70
1	X	1	DT	N1-C1'-C2'	5.26	122.59	112.60
3	N	35	DG	C8-N9-C4	-5.10	104.36	106.40
1	M	15	DT	C6-C5-C7	-5.09	119.84	122.90
1	M	12	DT	C5-C4-O4	-5.09	121.34	124.90
1	U	15	DT	C6-C5-C7	-5.08	119.85	122.90
3	Y	23	DT	P-O3'-C3'	5.07	125.78	119.70
1	U	9	DC	O4'-C1'-N1	5.05	111.53	108.00
1	U	19	DT	O4'-C1'-N1	5.04	111.53	108.00
1	X	15	DT	C6-C5-C7	-5.03	119.88	122.90
3	N	34	DT	C6-C5-C7	-5.03	119.88	122.90
1	J	12	DT	O4'-C1'-N1	5.01	111.51	108.00

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	J	385	0	219	3	0
1	M	385	0	219	11	0
1	U	385	0	219	10	0
1	X	385	0	219	20	0
2	I	63	0	34	1	0
2	O	63	0	34	1	0
2	W	63	0	34	2	0
2	Z	63	0	34	1	0
3	K	263	0	149	4	0
3	N	263	0	149	12	0
3	V	263	0	149	13	0
3	Y	263	0	149	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1422	0	1483	44	0
4	B	1414	0	1471	20	0
4	D	1414	0	1471	34	0
4	E	1422	0	1483	37	0
All	All	8516	0	7516	216	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 14.

All (216) 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)
3:Y:30:DA:H2"	3:Y:31:DC:H5"	1.27	1.15
3:N:28:DG:H2"	3:N:29:DG:H5"	1.29	1.12
3:Y:25:DA:H2"	3:Y:26:DT:H5"	1.34	1.07
1:X:2:DC:H2"	1:X:3:DA:OP2	1.52	1.05
3:N:30:DA:H2"	3:N:31:DC:H5"	1.46	0.95
3:Y:30:DA:C2'	3:Y:31:DC:H5"	2.05	0.84
4:B:118:GLU:HG3	4:B:121:ARG:HH21	1.43	0.83
4:B:70:GLY:HA3	4:B:76:MET:HG2	1.62	0.81
4:E:118:GLU:HG3	4:E:121:ARG:HH21	1.45	0.81
3:N:28:DG:C2'	3:N:29:DG:H5"	2.10	0.79
4:E:70:GLY:HA3	4:E:76:MET:HG2	1.63	0.79
1:M:5:DT:H2"	1:M:6:DG:H5"	1.65	0.77
4:A:11:THR:HG22	4:A:12:SER:H	1.50	0.76
3:Y:34:DT:H2'	3:Y:35:DG:C8	2.21	0.75
4:B:11:THR:HG22	4:B:12:SER:H	1.52	0.75
1:X:11:DA:H2"	1:X:12:DT:O5'	1.87	0.74
3:V:26:DT:H2"	3:V:27:DC:H5"	1.69	0.74
3:N:34:DT:H2"	3:N:35:DG:O4'	1.87	0.73
1:U:2:DC:H3'	1:U:3:DA:C8	2.23	0.72
1:X:1:DT:C2	1:X:2:DC:H5"	2.24	0.72
4:D:11:THR:HG22	4:D:12:SER:H	1.54	0.72
4:E:11:THR:HG22	4:E:12:SER:H	1.56	0.70
3:N:33:DC:H2"	3:N:34:DT:H5'	1.72	0.70
3:N:34:DT:H2"	3:N:35:DG:C8	2.27	0.69
4:A:78:GLN:O	4:A:82:GLU:HG2	1.92	0.68
3:V:30:DA:H2"	3:V:31:DC:H5"	1.75	0.68
1:M:5:DT:H2"	1:M:6:DG:C5'	2.25	0.67
3:Y:27:DC:H2"	3:Y:28:DG:O5'	1.94	0.67
3:Y:25:DA:H2"	3:Y:26:DT:C5'	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:ASP:OD2	4:A:75:ASP:HB3	1.96	0.65
4:E:52:ARG:NH1	4:E:82:GLU:OE1	2.29	0.65
3:V:34:DT:C2'	3:V:35:DG:C8	2.80	0.64
4:E:130:ARG:O	4:E:134:MET:HB2	1.98	0.64
3:V:34:DT:H2'	3:V:35:DG:C8	2.33	0.64
3:K:33:DC:H2"	3:K:34:DT:H5"	1.80	0.63
4:D:118:GLU:HG3	4:D:121:ARG:HH21	1.64	0.62
4:B:70:GLY:HA3	4:B:76:MET:CG	2.28	0.61
3:K:32:DA:H2"	3:K:33:DC:H5"	1.83	0.61
3:V:28:DG:H2"	3:V:29:DG:H5"	1.83	0.61
4:A:43:SER:HB3	4:A:71:ARG:HH22	1.66	0.60
3:V:32:DA:H2"	3:V:33:DC:H5"	1.83	0.60
1:M:4:DG:C2	3:N:34:DT:O2	2.54	0.60
4:A:43:SER:CB	4:A:71:ARG:HH22	2.14	0.60
1:M:8:DC:H2"	1:M:9:DC:O5'	2.01	0.60
1:X:9:DC:H2"	1:X:10:DG:C8	2.37	0.59
3:Y:25:DA:C2'	3:Y:26:DT:H5"	2.22	0.59
4:B:9:VAL:HG21	4:B:14:GLN:HA	1.85	0.58
1:X:2:DC:C2'	1:X:3:DA:OP2	2.39	0.58
3:K:30:DA:H2"	3:K:31:DC:H5"	1.86	0.57
4:A:11:THR:HG22	4:A:12:SER:N	2.19	0.57
1:M:9:DC:H2"	1:M:10:DG:C8	2.39	0.57
3:V:26:DT:H2"	3:V:27:DC:C5'	2.34	0.57
4:A:16:LEU:O	4:A:20:VAL:HG23	2.05	0.57
4:E:78:GLN:O	4:E:82:GLU:HG3	2.05	0.57
4:D:118:GLU:O	4:D:122:ILE:HG12	2.05	0.57
4:E:9:VAL:HG21	4:E:14:GLN:HA	1.87	0.57
3:Y:26:DT:H3'	4:A:146:ILE:HD11	1.86	0.56
4:A:9:VAL:HG21	4:A:14:GLN:HA	1.87	0.56
1:X:10:DG:H1'	1:X:11:DA:H5"	1.87	0.56
1:U:10:DG:H1'	1:U:11:DA:H5"	1.87	0.56
4:E:98:SER:OG	4:E:100:ASP:HB2	2.04	0.56
4:B:11:THR:HG22	4:B:12:SER:N	2.19	0.56
1:X:3:DA:H2"	1:X:4:DG:OP2	2.06	0.56
4:E:131:GLN:C	4:E:133:ALA:H	2.09	0.55
4:D:11:THR:HG22	4:D:12:SER:N	2.20	0.55
4:A:149:ASP:O	4:A:153:ASN:HB2	2.06	0.55
4:D:9:VAL:HG21	4:D:14:GLN:HA	1.86	0.55
2:I:20:DA:H5'	4:B:10:SER:HB2	1.87	0.55
2:W:20:DA:H5'	4:E:10:SER:HB2	1.89	0.55
4:A:99:THR:HG22	4:A:99:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:34:DT:H2"	3:V:35:DG:C8	2.40	0.55
4:A:69:LEU:HD23	4:A:76:MET:HG3	1.89	0.55
4:D:14:GLN:C	4:D:16:LEU:H	2.11	0.54
3:V:35:DG:H5"	3:V:35:DG:H8	1.73	0.54
1:J:3:DA:H2"	1:J:4:DG:OP2	2.08	0.54
4:E:11:THR:HG22	4:E:12:SER:N	2.22	0.53
4:A:90:ILE:H	4:A:99:THR:HB	1.72	0.53
3:N:29:DG:H2"	3:N:30:DA:C8	2.44	0.53
1:X:8:DC:H2"	1:X:9:DC:O5'	2.07	0.53
4:A:130:ARG:O	4:A:134:MET:HB2	2.08	0.53
4:B:78:GLN:O	4:B:82:GLU:HG3	2.09	0.53
4:A:2:ALA:HB3	4:A:59:ASP:OD1	2.08	0.53
4:A:127:ASN:HA	4:A:130:ARG:HG3	1.90	0.53
1:X:2:DC:H42	3:Y:35:DG:H22	1.57	0.53
3:K:25:DA:H1'	3:K:26:DT:H5"	1.89	0.53
1:X:18:DA:H2'	1:X:19:DT:C6	2.45	0.52
1:U:9:DC:H2'	1:U:10:DG:C8	2.45	0.52
4:D:78:GLN:O	4:D:82:GLU:HG2	2.09	0.52
4:D:66:LEU:HD21	4:D:108:VAL:HG13	1.91	0.51
3:Y:34:DT:H2"	3:Y:35:DG:O4'	2.10	0.51
4:A:83:PHE:HB3	4:A:88:VAL:HG23	1.92	0.51
4:D:86:GLN:HG2	4:D:86:GLN:O	2.10	0.51
4:E:98:SER:C	4:E:100:ASP:H	2.14	0.51
4:E:177:LYS:O	4:E:181:GLU:HB2	2.11	0.51
3:N:32:DA:H2"	3:N:33:DC:H5"	1.91	0.51
4:A:45:ARG:HD3	4:A:71:ARG:HH21	1.76	0.50
1:M:2:DC:O2	1:M:2:DC:C2'	2.59	0.50
4:E:8:ARG:H	4:E:19:GLN:HE22	1.59	0.50
3:Y:33:DC:C5'	3:Y:33:DC:H6	2.25	0.49
1:U:2:DC:H2'	1:U:2:DC:O2	2.11	0.49
1:X:6:DG:N7	4:A:172:ARG:NH2	2.61	0.49
4:B:98:SER:OG	4:B:100:ASP:HB2	2.13	0.49
4:E:8:ARG:O	4:E:19:GLN:NE2	2.45	0.49
4:E:59:ASP:HB2	4:E:88:VAL:HG12	1.95	0.49
4:E:83:PHE:HD2	4:E:88:VAL:HG21	1.76	0.48
4:D:2:ALA:HB3	4:D:59:ASP:OD1	2.13	0.48
4:A:14:GLN:C	4:A:16:LEU:H	2.16	0.48
3:V:27:DC:H5'	3:V:27:DC:H6	1.78	0.48
4:E:83:PHE:HB3	4:E:88:VAL:HG23	1.94	0.48
4:A:76:MET:HG2	4:A:76:MET:O	2.14	0.48
4:A:126:THR:O	4:A:130:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:20:DA:H5'	4:A:10:SER:HB2	1.95	0.48
4:B:14:GLN:C	4:B:16:LEU:H	2.18	0.48
4:A:99:THR:CG2	4:A:99:THR:O	2.62	0.48
1:X:1:DT:N1	1:X:2:DC:H5"	2.28	0.47
1:X:1:DT:H2"	1:X:2:DC:OP2	2.14	0.47
4:E:83:PHE:CD2	4:E:88:VAL:HG21	2.49	0.47
4:A:38:ALA:C	4:A:40:GLY:H	2.18	0.47
1:X:3:DA:OP2	1:X:3:DA:C8	2.67	0.47
4:B:15:SER:C	4:B:17:ASP:N	2.66	0.47
3:V:26:DT:C2'	3:V:27:DC:H5"	2.43	0.47
4:A:13:GLN:O	4:A:13:GLN:HG2	2.15	0.47
4:A:73:THR:N	4:A:116:GLN:OE1	2.42	0.47
4:B:13:GLN:HG2	4:B:13:GLN:O	2.15	0.47
4:A:65:LYS:HE2	4:A:94:ASP:OD2	2.14	0.46
4:A:6:TYR:CE1	4:A:48:LEU:HB2	2.50	0.46
1:M:3:DA:H1'	1:M:4:DG:H8	1.80	0.46
4:D:20:VAL:HG13	4:D:33:ILE:HG21	1.98	0.46
4:B:131:GLN:HE22	4:B:134:MET:HG2	1.80	0.46
4:E:62:LEU:HD23	4:E:93:ILE:HD11	1.97	0.46
1:U:2:DC:C2'	1:U:2:DC:O2	2.63	0.46
4:D:103:ILE:O	4:D:107:VAL:HG23	2.15	0.46
3:Y:29:DG:H2"	3:Y:30:DA:C8	2.50	0.46
1:X:1:DT:H1'	1:X:2:DC:H5"	1.96	0.46
4:D:13:GLN:HG2	4:D:13:GLN:O	2.16	0.46
4:B:45:ARG:NH2	4:B:75:ASP:OD2	2.49	0.46
4:E:13:GLN:HG2	4:E:13:GLN:O	2.16	0.45
4:D:69:LEU:HD21	4:D:90:ILE:HD13	1.96	0.45
3:Y:30:DA:C3'	3:Y:31:DC:H5"	2.44	0.45
3:Y:32:DA:H2"	3:Y:33:DC:H5"	1.99	0.45
4:D:151:VAL:HG22	4:D:168:MET:HE3	1.98	0.45
1:U:6:DG:N7	4:E:172:ARG:NH2	2.64	0.45
3:Y:30:DA:H2"	3:Y:31:DC:C5'	2.19	0.45
1:U:2:DC:C3'	1:U:3:DA:C8	2.97	0.45
3:V:29:DG:H2"	3:V:30:DA:C8	2.52	0.45
4:A:6:TYR:HE1	4:A:48:LEU:HB2	1.82	0.45
4:A:155:TRP:C	4:A:157:GLN:H	2.20	0.45
4:E:6:TYR:CD2	4:E:6:TYR:C	2.90	0.45
4:E:43:SER:HB2	4:E:71:ARG:HH22	1.81	0.45
4:B:6:TYR:C	4:B:6:TYR:CD2	2.90	0.45
4:E:70:GLY:HA3	4:E:76:MET:CG	2.41	0.44
2:W:20:DA:C5'	4:E:10:SER:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:77:ILE:HD11	4:A:109:THR:HG23	1.99	0.44
1:X:4:DG:H2"	1:X:5:DT:H5"	2.00	0.44
4:A:11:THR:CG2	4:A:12:SER:H	2.27	0.44
4:E:6:TYR:HE1	4:E:48:LEU:HB2	1.82	0.44
4:D:6:TYR:C	4:D:6:TYR:CD2	2.90	0.44
4:B:11:THR:CG2	4:B:12:SER:H	2.28	0.44
1:M:12:DT:H2"	1:M:13:DA:C8	2.53	0.44
4:D:123:LEU:O	4:D:127:ASN:HB2	2.18	0.44
4:E:6:TYR:CE1	4:E:48:LEU:HB2	2.53	0.44
1:M:15:DT:H5"	4:D:142:ARG:HA	2.00	0.44
4:A:75:ASP:C	4:A:75:ASP:OD1	2.56	0.43
1:X:19:DT:OP1	1:X:19:DT:H4'	2.19	0.43
4:D:136:LYS:N	4:D:136:LYS:HD2	2.34	0.43
4:A:6:TYR:CD2	4:A:6:TYR:C	2.91	0.43
1:X:1:DT:H1'	1:X:2:DC:C5'	2.49	0.43
4:A:116:GLN:HB3	4:A:116:GLN:HE21	1.67	0.43
4:D:159:LEU:HD22	4:D:163:HIS:CD2	2.53	0.43
4:D:164:ILE:HG23	4:D:168:MET:HE2	1.99	0.43
3:N:24:DT:H2"	3:N:25:DA:C8	2.54	0.43
4:A:71:ARG:HG3	4:A:71:ARG:H	1.55	0.43
4:B:16:LEU:O	4:B:20:VAL:HG23	2.19	0.43
4:D:98:SER:C	4:D:100:ASP:H	2.21	0.43
1:X:4:DG:H2"	1:X:5:DT:C5'	2.49	0.43
4:A:78:GLN:O	4:A:82:GLU:CG	2.65	0.43
4:E:84:ASP:OD2	4:E:105:LYS:HE2	2.19	0.43
4:E:73:THR:O	4:E:77:ILE:HG13	2.18	0.42
1:U:18:DA:H2"	1:U:19:DT:C6	2.54	0.42
1:J:2:DC:H2'	1:J:3:DA:C4	2.54	0.42
1:M:1:DT:O3'	1:M:2:DC:H4'	2.20	0.42
1:M:4:DG:N2	3:N:34:DT:O2	2.53	0.42
2:O:20:DA:H5'	4:D:10:SER:HB2	2.01	0.42
4:A:110:ILE:O	4:A:114:VAL:HG23	2.20	0.42
1:X:3:DA:OP2	1:X:3:DA:H2'	2.20	0.42
4:D:8:ARG:O	4:D:19:GLN:NE2	2.52	0.42
1:U:1:DT:H2"	1:U:2:DC:H4'	2.01	0.42
4:E:80:ILE:O	4:E:84:ASP:HB2	2.20	0.42
4:E:84:ASP:C	4:E:86:GLN:H	2.24	0.42
1:U:17:DT:H5'	4:E:140:PHE:CE2	2.55	0.42
4:D:11:THR:CG2	4:D:12:SER:H	2.29	0.42
4:E:14:GLN:C	4:E:16:LEU:H	2.24	0.42
4:D:83:PHE:CD1	4:D:90:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:LYS:HE3	4:D:181:GLU:OE2	2.20	0.42
4:D:66:LEU:C	4:D:68:ARG:H	2.24	0.41
4:A:66:LEU:C	4:A:68:ARG:H	2.23	0.41
3:Y:33:DC:H5"	3:Y:33:DC:H6	1.84	0.41
4:D:151:VAL:HG22	4:D:168:MET:CE	2.50	0.41
4:D:70:GLY:HA3	4:D:76:MET:HG2	2.02	0.41
4:A:146:ILE:HD12	4:A:174:THR:HG21	2.02	0.41
4:D:71:ARG:HG3	4:D:71:ARG:H	1.64	0.41
3:N:32:DA:C2'	3:N:33:DC:H5"	2.51	0.41
4:D:43:SER:CB	4:D:71:ARG:HH22	2.34	0.41
4:A:154:MET:HG2	4:A:159:LEU:HD12	2.03	0.41
4:A:41:SER:O	4:A:42:SER:C	2.58	0.41
4:D:6:TYR:HE1	4:D:48:LEU:HB2	1.86	0.41
4:B:66:LEU:HD21	4:B:108:VAL:HG13	2.01	0.41
3:V:35:DG:H5"	3:V:35:DG:C8	2.56	0.40
4:E:66:LEU:C	4:E:68:ARG:H	2.24	0.40
4:B:83:PHE:HB3	4:B:88:VAL:HG22	2.03	0.40
4:E:65:LYS:HG2	4:E:66:LEU:H	1.86	0.40
4:E:11:THR:CG2	4:E:12:SER:H	2.31	0.40
4:B:4:PHE:O	4:B:62:LEU:N	2.51	0.40
4:A:111:LEU:HD23	4:A:111:LEU:HA	1.69	0.40
4:D:6:TYR:CE1	4:D:48:LEU:HB2	2.56	0.40
1:J:10:DG:H2"	1:J:11:DA:H5"	2.03	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
4	A	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	5 37
4	B	180/183 (98%)	154 (86%)	23 (13%)	3 (2%)	11 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	180/183 (98%)	155 (86%)	22 (12%)	3 (2%)	11 51
4	E	181/183 (99%)	153 (84%)	24 (13%)	4 (2%)	8 46
All	All	722/732 (99%)	621 (86%)	85 (12%)	16 (2%)	8 46

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	31	ASN
4	E	42	SER
4	A	31	ASN
4	A	39	SER
4	A	99	THR
4	A	38	ALA
4	A	67	ASP
4	D	42	SER
4	A	42	SER
4	B	42	SER
4	E	132	GLU
4	B	16	LEU
4	E	67	ASP
4	D	67	ASP
4	E	93	ILE
4	D	93	ILE

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
4	A	153/153 (100%)	139 (91%)	14 (9%)	11 43
4	B	152/153 (99%)	135 (89%)	17 (11%)	7 32
4	D	152/153 (99%)	137 (90%)	15 (10%)	10 39
4	E	153/153 (100%)	142 (93%)	11 (7%)	18 56
All	All	610/612 (100%)	553 (91%)	57 (9%)	11 42

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	12	SER
4	A	32	ARG
4	A	35	THR
4	A	36	ASP
4	A	68	ARG
4	A	72	ASP
4	A	75	ASP
4	A	82	GLU
4	A	100	ASP
4	A	106	MET
4	A	116	GLN
4	A	130	ARG
4	A	153	ASN
4	A	165	SER
4	B	12	SER
4	B	35	THR
4	B	36	ASP
4	B	41	SER
4	B	50	LEU
4	B	53	MET
4	B	63	VAL
4	B	72	ASP
4	B	76	MET
4	B	79	LEU
4	B	88	VAL
4	B	97	ILE
4	B	118	GLU
4	B	119	ARG
4	B	123	LEU
4	B	169	ASN
4	B	174	THR
4	E	12	SER
4	E	36	ASP
4	E	50	LEU
4	E	54	LYS
4	E	63	VAL
4	E	72	ASP
4	E	76	MET
4	E	103	ILE
4	E	118	GLU
4	E	162	SER
4	E	174	THR

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Mol	Chain	Res	Type
4	D	12	SER
4	D	36	ASP
4	D	49	ASP
4	D	50	LEU
4	D	71	ARG
4	D	72	ASP
4	D	76	MET
4	D	82	GLU
4	D	103	ILE
4	D	118	GLU
4	D	119	ARG
4	D	123	LEU
4	D	127	ASN
4	D	136	LYS
4	D	162	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	131	GLN
4	B	169	ASN
4	B	183	ASN
4	E	120	GLN
4	E	127	ASN
4	E	163	HIS
4	D	163	HIS
4	D	169	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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	J	19/19 (100%)	1.50	6 (31%) 1 1	116, 121, 156, 175	0
1	M	19/19 (100%)	0.57	2 (10%) 8 8	107, 121, 166, 180	0
1	U	19/19 (100%)	0.82	2 (10%) 8 8	116, 121, 159, 177	0
1	X	19/19 (100%)	-0.26	1 (5%) 30 27	108, 113, 133, 151	0
2	I	3/3 (100%)	0.20	0 100 100	86, 86, 105, 119	0
2	O	3/3 (100%)	-0.42	0 100 100	85, 85, 105, 120	0
2	W	3/3 (100%)	-0.57	0 100 100	86, 86, 105, 120	0
2	Z	3/3 (100%)	-0.41	0 100 100	86, 86, 104, 119	0
3	K	13/13 (100%)	2.18	4 (30%) 1 1	116, 119, 121, 122	0
3	N	13/13 (100%)	0.41	1 (7%) 16 16	112, 119, 130, 137	0
3	V	13/13 (100%)	-0.04	0 100 100	115, 120, 123, 135	0
3	Y	13/13 (100%)	-0.38	0 100 100	100, 111, 117, 117	0
4	A	183/183 (100%)	0.37	6 (3%) 50 45	67, 100, 137, 221	0
4	B	182/183 (99%)	1.06	38 (20%) 1 1	68, 106, 141, 221	0
4	D	182/183 (99%)	0.29	10 (5%) 29 26	68, 106, 135, 221	0
4	E	183/183 (100%)	0.52	18 (9%) 10 10	68, 106, 140, 221	0
All	All	870/872 (99%)	0.56	88 (10%) 9 9	67, 108, 140, 221	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	1	DT	15.5
4	B	151	VAL	10.1
3	K	33	DC	8.6
4	B	146	ILE	8.5
3	K	32	DA	8.4

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Mol	Chain	Res	Type	RSRZ
1	J	6	DG	7.3
1	J	1	DT	7.0
4	B	147	ASP	6.9
4	B	150	ALA	6.9
4	B	42	SER	6.5
4	B	161	ALA	6.4
4	E	40	GLY	6.3
4	B	149	ASP	6.2
4	B	148	ARG	6.1
1	M	1	DT	6.0
4	B	153	ASN	5.4
4	B	165	SER	5.3
4	A	39	SER	5.0
4	A	155	TRP	4.7
4	D	183	ASN	4.7
3	N	35	DG	4.7
4	E	153	ASN	4.6
3	K	31	DC	4.5
4	B	164	ILE	4.5
4	E	39	SER	4.5
4	E	157	GLN	4.4
4	B	155	TRP	4.2
4	B	158	GLY	4.2
4	B	162	SER	4.2
4	E	1	MET	4.0
4	B	145	LYS	4.0
4	B	177	LYS	4.0
4	D	156	GLN	3.8
4	A	153	ASN	3.7
4	B	179	ILE	3.7
4	B	152	LEU	3.7
4	B	178	VAL	3.7
1	J	5	DT	3.7
4	E	42	SER	3.6
4	B	154	MET	3.6
4	B	39	SER	3.6
3	K	35	DG	3.6
1	J	8	DC	3.6
4	B	156	GLN	3.5
4	B	14	GLN	3.5
4	B	163	HIS	3.5
4	B	181	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
4	B	172	ARG	3.3
1	M	2	DC	3.2
4	A	40	GLY	3.2
4	B	173	SER	3.2
4	E	167	THR	3.2
4	E	149	ASP	3.2
4	B	182	SER	3.2
4	B	168	MET	3.1
4	E	155	TRP	3.1
4	D	152	LEU	2.9
1	J	7	DT	2.8
4	E	132	GLU	2.8
4	B	176	TYR	2.7
4	D	151	VAL	2.7
1	J	4	DG	2.6
4	B	140	PHE	2.6
4	E	151	VAL	2.5
4	D	69	LEU	2.4
4	B	183	ASN	2.4
4	E	168	MET	2.4
4	D	14	GLN	2.3
4	B	38	ALA	2.3
4	B	43	SER	2.3
4	D	29	LYS	2.3
1	U	3	DA	2.3
4	E	181	GLU	2.3
4	D	155	TRP	2.3
4	A	14	GLN	2.3
4	B	166	LYS	2.2
4	E	14	GLN	2.2
4	D	168	MET	2.2
1	X	1	DT	2.2
4	B	26	ALA	2.2
4	B	9	VAL	2.2
4	E	183	ASN	2.2
4	D	174	THR	2.1
4	E	159	LEU	2.1
4	A	140	PHE	2.1
4	E	41	SER	2.0
4	E	101	SER	2.0
4	B	175	VAL	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.