Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 04:34 PM EDT

PDB ID	:	2EX5
Title	:	Group I Intron-encoded Homing Endonuclease I-CeuI Complexed With DNA
Authors	:	Spiegel, P.C.; Stoddard, B.L.
Deposited on	:	2005-11-07
Resolution	:	2.20 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 following versions of software and data (see references (1)) were used in the production of this report:

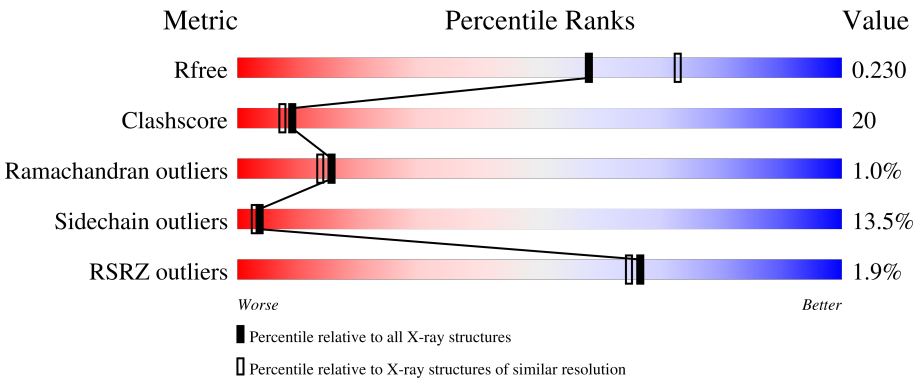
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	X	26	35% 65%
2	Y	26	4% • 27% 69%
3	A	207	2% 60% 33% 6%
3	B	207	2% 61% 29% 6% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4664 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 I-CeuI DNA target site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	26	535	254	106	150	25	0	0	0

- Molecule 2 is a DNA chain called I-CeuI DNA target site, complementary strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	26	525	252	90	158	25	0	0	0

- Molecule 3 is a protein called DNA endonuclease I-CeuI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	207	1669	1071	286	311	1	0	0	0
3	B	207	1669	1071	286	311	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ARG	GLN	engineered mutation	UNP P32761
B	93	ARG	GLN	engineered mutation	UNP P32761

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	X	27	27	27	0	0
			Total	O		
5	Y	40	40	40	0	0
			Total	O		
5	A	118	118	118	0	0
			Total	O		
5	B	78	78	78	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: I-CeuI DNA target site

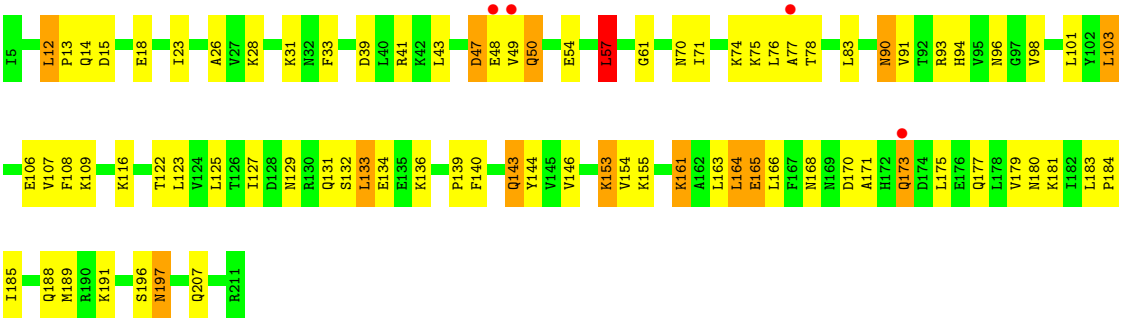
Chain X: 35% 65%

• Molecule 2: I-CeuI DNA target site, complementary strand

Chain Y: 4% 27% 69%

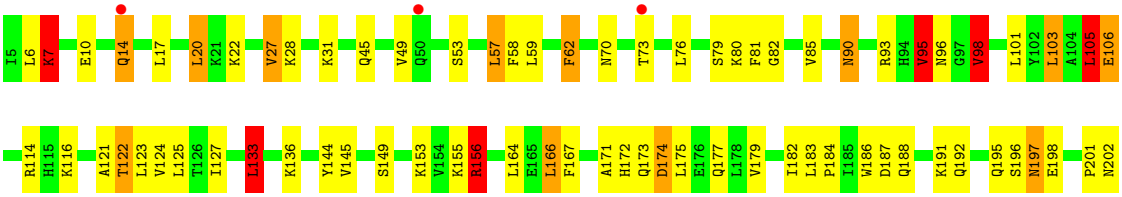
• Molecule 3: DNA endonuclease I-CeuI

Chain A: 2% 60% 33% 6%



• Molecule 3: DNA endonuclease I-CeuI

Chain B: 2% 61% 29% 6%



L203
E204
A205
A206
Q207
D208
F209
A210
R211

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.23Å 69.18Å 169.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.20) 96.4 (19.83-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.231 0.218 , 0.230	Depositor DCC
R_{free} test set	3057 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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: CA

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	X	2.23	24/602 (4.0%)	3.33	122/928 (13.1%)
2	Y	2.41	29/586 (4.9%)	3.54	135/902 (15.0%)
3	A	1.46	12/1697 (0.7%)	1.21	9/2283 (0.4%)
3	B	1.24	4/1697 (0.2%)	1.15	9/2283 (0.4%)
All	All	1.66	69/4582 (1.5%)	2.09	275/6396 (4.3%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	606	DA	N7-C5	9.68	1.45	1.39
2	Y	714	DA	N3-C4	9.52	1.40	1.34
1	X	609	DG	C6-N1	8.65	1.45	1.39
2	Y	701	DG	C8-N7	8.27	1.35	1.30
1	X	618	DT	N1-C6	8.00	1.43	1.38
2	Y	706	DG	N7-C5	7.96	1.44	1.39
1	X	604	DT	C5-C7	7.92	1.54	1.50
1	X	611	DC	C2-N3	7.88	1.42	1.35
3	A	91	VAL	CB-CG1	7.84	1.69	1.52
2	Y	721	DT	N3-C4	-7.42	1.32	1.38
3	A	140	PHE	CG-CD1	7.34	1.49	1.38
2	Y	716	DG	O3'-P	-7.23	1.52	1.61
2	Y	714	DA	N1-C2	7.22	1.40	1.34
1	X	611	DC	C2-O2	7.21	1.30	1.24
1	X	606	DA	N9-C8	7.12	1.43	1.37
2	Y	704	DT	C1'-N1	7.10	1.58	1.49
2	Y	701	DG	C6-N1	7.09	1.44	1.39
2	Y	720	DG	C5-C4	-7.03	1.33	1.38
3	B	106	GLU	CG-CD	-6.99	1.41	1.51
2	Y	714	DA	C2-N3	6.91	1.39	1.33
2	Y	716	DG	C3'-O3'	6.84	1.52	1.44
3	B	191	LYS	CE-NZ	6.80	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	707	DC	N3-C4	6.54	1.38	1.33
2	Y	708	DT	C5-C7	6.50	1.53	1.50
1	X	626	DC	C1'-N1	6.48	1.57	1.49
2	Y	718	DC	C1'-N1	6.46	1.57	1.49
1	X	612	DC	C3'-O3'	-6.43	1.35	1.44
1	X	612	DC	C4-C5	6.42	1.48	1.43
3	A	134	GLU	CB-CG	-6.39	1.40	1.52
1	X	609	DG	C2-N2	6.31	1.40	1.34
3	A	140	PHE	CE2-CZ	6.25	1.49	1.37
2	Y	702	DC	C3'-O3'	-6.22	1.35	1.44
1	X	611	DC	N1-C6	6.09	1.40	1.37
2	Y	708	DT	N1-C6	-6.09	1.33	1.38
1	X	609	DG	N7-C5	6.08	1.42	1.39
1	X	607	DC	N1-C6	-5.98	1.33	1.37
2	Y	718	DC	C5-C6	5.92	1.39	1.34
3	A	165	GLU	CG-CD	5.87	1.60	1.51
2	Y	716	DG	C6-N1	5.78	1.43	1.39
2	Y	710	DC	C2-N3	5.70	1.40	1.35
3	A	98	VAL	CB-CG1	5.69	1.64	1.52
1	X	614	DA	N7-C5	5.59	1.42	1.39
3	A	26	ALA	CA-CB	5.55	1.64	1.52
1	X	609	DG	C2-N3	5.50	1.37	1.32
2	Y	713	DT	C1'-N1	5.45	1.56	1.49
2	Y	716	DG	C5'-C4'	5.45	1.57	1.51
2	Y	719	DC	C1'-N1	5.43	1.56	1.49
2	Y	715	DG	N7-C5	5.41	1.42	1.39
1	X	606	DA	O4'-C1'	5.39	1.48	1.42
2	Y	716	DG	C4'-C3'	-5.37	1.47	1.52
3	A	140	PHE	CE1-CZ	5.33	1.47	1.37
1	X	616	DG	P-OP2	5.33	1.58	1.49
3	B	7	LYS	CD-CE	5.31	1.64	1.51
2	Y	717	DA	C3'-C2'	5.26	1.58	1.52
3	A	161	LYS	CE-NZ	5.24	1.62	1.49
2	Y	704	DT	N1-C2	5.24	1.42	1.38
3	A	91	VAL	CB-CG2	-5.22	1.41	1.52
2	Y	701	DG	N9-C8	5.21	1.41	1.37
3	A	33	PHE	CD1-CE1	5.20	1.49	1.39
1	X	601	DC	C2-N3	5.14	1.39	1.35
3	A	155	LYS	CD-CE	5.12	1.64	1.51
1	X	611	DC	N3-C4	5.09	1.37	1.33
1	X	607	DC	N3-C4	-5.06	1.30	1.33
1	X	613	DT	N1-C2	5.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	607	DC	C3'-O3'	-5.06	1.37	1.44
2	Y	717	DA	N7-C5	5.06	1.42	1.39
3	B	62	PHE	CE1-CZ	5.05	1.47	1.37
2	Y	714	DA	C3'-C2'	5.04	1.58	1.52
1	X	616	DG	N1-C2	-5.00	1.33	1.37

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	708	DT	C6-C5-C7	-16.84	112.80	122.90
1	X	607	DC	O4'-C1'-N1	16.67	119.67	108.00
1	X	601	DC	O4'-C1'-N1	-15.76	96.97	108.00
2	Y	704	DT	O4'-C1'-N1	12.31	116.62	108.00
1	X	603	DA	O4'-C1'-N9	12.20	116.54	108.00
2	Y	715	DG	C5-C6-N1	12.16	117.58	111.50
1	X	613	DT	C6-C5-C7	-12.03	115.68	122.90
2	Y	704	DT	N3-C2-O2	-12.03	115.08	122.30
1	X	604	DT	N3-C2-O2	-11.99	115.11	122.30
2	Y	718	DC	N1-C2-O2	-11.59	111.95	118.90
1	X	602	DG	N3-C2-N2	-11.27	112.01	119.90
2	Y	701	DG	N3-C4-N9	-11.17	119.30	126.00
1	X	615	DA	P-O5'-C5'	-10.75	103.70	120.90
1	X	607	DC	O5'-P-OP1	-10.75	96.03	105.70
2	Y	724	DT	C6-C5-C7	-10.74	116.45	122.90
2	Y	708	DT	C4-C5-C7	10.66	125.40	119.00
2	Y	709	DA	N1-C2-N3	-10.66	123.97	129.30
2	Y	720	DG	P-O3'-C3'	10.32	132.09	119.70
2	Y	715	DG	C5-C6-O6	-10.28	122.43	128.60
2	Y	721	DT	C5-C6-N1	-10.04	117.67	123.70
2	Y	726	DG	O4'-C1'-N9	10.00	115.00	108.00
2	Y	726	DG	N1-C6-O6	-9.89	113.96	119.90
2	Y	713	DT	C6-C5-C7	-9.88	116.97	122.90
1	X	614	DA	C5-C6-N6	9.80	131.54	123.70
2	Y	716	DG	C2-N3-C4	9.67	116.73	111.90
2	Y	716	DG	O4'-C1'-C2'	-9.66	98.17	105.90
2	Y	703	DT	N3-C4-O4	9.62	125.67	119.90
1	X	606	DA	O4'-C1'-C2'	-9.54	98.26	105.90
2	Y	723	DA	C5'-C4'-C3'	-9.46	97.07	114.10
2	Y	722	DT	P-O3'-C3'	9.45	131.04	119.70
1	X	608	DG	P-O3'-C3'	9.39	130.97	119.70
2	Y	710	DC	O4'-C1'-N1	9.25	114.48	108.00
1	X	609	DG	C2-N3-C4	9.24	116.52	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	618	DT	O4'-C4'-C3'	-9.21	100.47	106.00
1	X	623	DA	O4'-C4'-C3'	-9.15	100.51	106.00
1	X	622	DG	N3-C2-N2	-9.14	113.50	119.90
1	X	612	DC	O4'-C1'-N1	9.11	114.38	108.00
1	X	617	DG	O4'-C1'-C2'	-9.07	98.64	105.90
2	Y	716	DG	N3-C2-N2	-9.05	113.56	119.90
2	Y	714	DA	P-O3'-C3'	9.04	130.54	119.70
1	X	602	DG	N1-C6-O6	8.97	125.28	119.90
1	X	613	DT	O4'-C1'-N1	8.96	114.28	108.00
2	Y	704	DT	O4'-C1'-C2'	-8.93	98.75	105.90
2	Y	715	DG	C5'-C4'-O4'	-8.86	92.46	109.30
2	Y	716	DG	C5-C6-O6	-8.76	123.34	128.60
2	Y	712	DT	N3-C4-O4	8.72	125.14	119.90
1	X	609	DG	N1-C6-O6	-8.64	114.71	119.90
1	X	614	DA	C5'-C4'-C3'	-8.64	98.54	114.10
2	Y	716	DG	C8-N9-C4	-8.63	102.95	106.40
1	X	614	DA	N1-C6-N6	-8.57	113.46	118.60
2	Y	712	DT	C5-C4-O4	-8.48	118.96	124.90
1	X	602	DG	O4'-C1'-N9	8.48	113.94	108.00
2	Y	716	DG	N1-C2-N2	8.46	123.82	116.20
1	X	604	DT	P-O3'-C3'	8.42	129.80	119.70
2	Y	724	DT	C4-C5-C7	8.34	124.00	119.00
2	Y	703	DT	C5-C4-O4	-8.31	119.08	124.90
2	Y	701	DG	N9-C4-C5	8.27	108.71	105.40
2	Y	715	DG	O5'-P-OP1	-8.27	98.26	105.70
2	Y	713	DT	O4'-C1'-N1	8.23	113.76	108.00
2	Y	717	DA	O4'-C1'-N9	8.22	113.75	108.00
2	Y	705	DC	N3-C4-N4	-8.19	112.26	118.00
1	X	611	DC	OP1-P-OP2	8.16	131.84	119.60
1	X	606	DA	C5-N7-C8	-7.96	99.92	103.90
2	Y	721	DT	O4'-C1'-C2'	7.95	112.26	105.90
1	X	615	DA	O4'-C1'-N9	-7.87	102.49	108.00
2	Y	712	DT	O4'-C1'-N1	-7.83	102.52	108.00
1	X	611	DC	O5'-P-OP2	-7.82	98.66	105.70
2	Y	715	DG	P-O5'-C5'	7.82	133.41	120.90
1	X	618	DT	P-O5'-C5'	7.79	133.36	120.90
1	X	605	DA	O3'-P-O5'	7.77	118.77	104.00
2	Y	709	DA	C2-N3-C4	7.76	114.48	110.60
2	Y	715	DG	C6-N1-C2	-7.76	120.44	125.10
1	X	620	DG	N3-C2-N2	-7.75	114.48	119.90
1	X	609	DG	O4'-C1'-N9	7.74	113.42	108.00
2	Y	726	DG	N9-C4-C5	7.73	108.49	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	722	DT	N3-C2-O2	-7.68	117.69	122.30
1	X	617	DG	O4'-C1'-N9	-7.68	102.63	108.00
2	Y	714	DA	O3'-P-O5'	7.67	118.58	104.00
1	X	618	DT	O4'-C1'-N1	7.67	113.37	108.00
2	Y	706	DG	N1-C6-O6	-7.61	115.33	119.90
2	Y	724	DT	O4'-C1'-N1	-7.61	102.67	108.00
2	Y	701	DG	C8-N9-C1'	7.60	136.88	127.00
1	X	602	DG	C5-C6-O6	-7.59	124.05	128.60
3	B	156	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	Y	716	DG	C6-N1-C2	-7.56	120.56	125.10
2	Y	719	DC	N3-C4-C5	-7.51	118.89	121.90
2	Y	718	DC	P-O5'-C5'	7.42	132.77	120.90
1	X	613	DT	C4-C5-C7	7.41	123.44	119.00
1	X	619	DA	N1-C2-N3	-7.41	125.60	129.30
1	X	606	DA	C1'-O4'-C4'	-7.38	102.72	110.10
2	Y	715	DG	N3-C4-N9	7.35	130.41	126.00
2	Y	726	DG	C5-C6-O6	7.33	133.00	128.60
1	X	611	DC	C5-C6-N1	7.30	124.65	121.00
1	X	609	DG	C5-C6-N1	7.29	115.15	111.50
1	X	613	DT	N3-C2-O2	-7.28	117.93	122.30
2	Y	705	DC	C5-C4-N4	7.25	125.28	120.20
2	Y	705	DC	C6-N1-C1'	7.25	129.50	120.80
3	B	98	VAL	CB-CA-C	-7.22	97.68	111.40
2	Y	711	DC	P-O3'-C3'	7.19	128.33	119.70
2	Y	715	DG	N9-C4-C5	-7.17	102.53	105.40
1	X	618	DT	C5-C6-N1	-7.15	119.41	123.70
2	Y	723	DA	P-O5'-C5'	-7.12	109.50	120.90
2	Y	715	DG	O4'-C1'-C2'	7.12	111.60	105.90
2	Y	719	DC	C2-N3-C4	7.12	123.46	119.90
2	Y	705	DC	C2-N1-C1'	-7.00	111.10	118.80
2	Y	721	DT	C4-C5-C6	6.94	122.17	118.00
3	B	156	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	X	607	DC	O5'-P-OP2	6.93	119.02	110.70
1	X	602	DG	N1-C2-N2	6.93	122.44	116.20
2	Y	716	DG	P-O5'-C5'	6.92	131.96	120.90
2	Y	701	DG	O4'-C4'-C3'	-6.85	101.76	104.50
2	Y	709	DA	O4'-C1'-C2'	-6.83	100.44	105.90
2	Y	720	DG	O4'-C1'-C2'	6.83	111.36	105.90
1	X	605	DA	O4'-C1'-N9	-6.82	103.22	108.00
1	X	610	DT	N3-C2-O2	-6.80	118.22	122.30
2	Y	707	DC	C4-C5-C6	6.79	120.80	117.40
2	Y	701	DG	N3-C4-C5	6.79	132.00	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	609	DG	C6-C5-N7	6.76	134.46	130.40
2	Y	716	DG	C5-C6-N1	6.73	114.86	111.50
2	Y	716	DG	O4'-C4'-C3'	-6.68	101.83	104.50
1	X	620	DG	P-O3'-C3'	6.56	127.57	119.70
3	B	133	LEU	CA-CB-CG	6.55	130.36	115.30
1	X	610	DT	C6-C5-C7	-6.52	118.99	122.90
2	Y	702	DC	C6-N1-C2	6.51	122.91	120.30
2	Y	714	DA	O4'-C4'-C3'	-6.51	101.90	104.50
1	X	609	DG	N3-C2-N2	6.50	124.45	119.90
2	Y	715	DG	C4-C5-N7	6.50	113.40	110.80
3	B	105	LEU	CB-CG-CD1	6.50	122.05	111.00
2	Y	704	DT	N1-C2-O2	6.47	128.27	123.10
1	X	618	DT	C2-N3-C4	-6.46	123.33	127.20
3	A	12	LEU	CA-CB-CG	6.46	130.15	115.30
2	Y	717	DA	O4'-C1'-C2'	-6.43	100.76	105.90
1	X	615	DA	O4'-C4'-C3'	6.42	109.85	106.00
2	Y	712	DT	N1-C2-O2	-6.40	117.98	123.10
1	X	603	DA	P-O5'-C5'	-6.38	110.70	120.90
2	Y	716	DG	C5'-C4'-O4'	6.37	121.40	109.30
2	Y	719	DC	C6-N1-C2	-6.32	117.77	120.30
2	Y	720	DG	O4'-C1'-N9	-6.28	103.60	108.00
1	X	614	DA	C5'-C4'-O4'	-6.26	97.40	109.30
1	X	607	DC	C4-C5-C6	6.24	120.52	117.40
1	X	602	DG	O4'-C4'-C3'	-6.22	102.01	104.50
1	X	614	DA	O5'-P-OP1	-6.20	100.12	105.70
2	Y	712	DT	P-O3'-C3'	6.16	127.10	119.70
1	X	619	DA	OP1-P-OP2	-6.16	110.36	119.60
2	Y	710	DC	N1-C2-O2	-6.14	115.22	118.90
1	X	626	DC	N3-C2-O2	-6.12	117.61	121.90
1	X	606	DA	C4-C5-N7	6.11	113.76	110.70
1	X	620	DG	C5-C6-O6	-6.10	124.94	128.60
1	X	609	DG	N1-C2-N3	-6.10	120.24	123.90
2	Y	721	DT	N3-C2-O2	6.08	125.95	122.30
1	X	625	DG	C5-C6-O6	-6.08	124.95	128.60
2	Y	712	DT	N1-C2-N3	6.08	118.25	114.60
1	X	604	DT	N1-C2-O2	6.07	127.95	123.10
1	X	601	DC	P-O3'-C3'	6.05	126.96	119.70
2	Y	703	DT	O4'-C1'-C2'	-6.03	101.08	105.90
2	Y	704	DT	P-O3'-C3'	6.03	126.93	119.70
1	X	609	DG	C4-C5-C6	-6.02	115.19	118.80
1	X	612	DC	C5-C4-N4	6.02	124.41	120.20
1	X	605	DA	C5-C6-N1	-6.01	114.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	726	DG	O4'-C4'-C3'	6.01	109.61	106.00
1	X	614	DA	C5-N7-C8	6.01	106.91	103.90
3	A	103	LEU	CA-CB-CG	6.01	129.11	115.30
1	X	613	DT	O4'-C1'-C2'	-5.99	101.11	105.90
1	X	617	DG	N1-C6-O6	-5.97	116.32	119.90
1	X	606	DA	OP1-P-O3'	5.96	118.32	105.20
1	X	615	DA	O5'-P-OP2	-5.94	100.35	105.70
2	Y	720	DG	O5'-P-OP1	-5.94	100.35	105.70
2	Y	708	DT	O4'-C1'-N1	-5.93	103.85	108.00
1	X	612	DC	N3-C4-N4	-5.92	113.85	118.00
1	X	612	DC	C4'-C3'-C2'	5.89	108.40	103.10
3	A	57	LEU	CA-CB-CG	5.88	128.82	115.30
3	B	95	VAL	CB-CA-C	-5.88	100.23	111.40
2	Y	702	DC	C4'-C3'-C2'	5.86	108.38	103.10
1	X	615	DA	O3'-P-O5'	-5.84	92.90	104.00
2	Y	704	DT	N3-C4-O4	5.83	123.40	119.90
2	Y	715	DG	C1'-O4'-C4'	-5.83	104.27	110.10
1	X	622	DG	C5-C6-O6	-5.82	125.11	128.60
1	X	625	DG	C5'-C4'-O4'	-5.81	98.27	109.30
1	X	604	DT	O4'-C1'-N1	5.81	112.06	108.00
1	X	612	DC	C2-N1-C1'	-5.79	112.43	118.80
2	Y	701	DG	C4-N9-C1'	-5.79	118.98	126.50
1	X	603	DA	N1-C2-N3	-5.79	126.41	129.30
2	Y	723	DA	C5-C6-N6	5.79	128.33	123.70
2	Y	712	DT	C2-N3-C4	-5.78	123.73	127.20
1	X	618	DT	OP2-P-O3'	5.77	117.90	105.20
1	X	615	DA	P-O3'-C3'	5.76	126.61	119.70
2	Y	710	DC	N3-C2-O2	5.76	125.93	121.90
2	Y	721	DT	C5'-C4'-C3'	-5.76	103.73	114.10
1	X	610	DT	C2-N3-C4	-5.76	123.75	127.20
2	Y	701	DG	C8-N9-C4	-5.76	104.10	106.40
2	Y	706	DG	C2-N3-C4	5.76	114.78	111.90
3	A	41	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	Y	721	DT	O4'-C4'-C3'	5.75	109.45	106.00
1	X	604	DT	C1'-O4'-C4'	-5.74	104.36	110.10
1	X	606	DA	O5'-P-OP1	-5.73	100.54	105.70
3	A	164	LEU	CA-CB-CG	5.72	128.46	115.30
1	X	616	DG	O4'-C1'-N9	5.71	112.00	108.00
1	X	613	DT	C4'-C3'-C2'	-5.70	97.97	103.10
1	X	614	DA	C6-C5-N7	5.70	136.29	132.30
2	Y	723	DA	N1-C6-N6	-5.69	115.19	118.60
1	X	614	DA	N7-C8-N9	-5.66	110.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	612	DC	C6-N1-C1'	5.66	127.59	120.80
2	Y	721	DT	C2-N1-C1'	-5.65	109.15	118.20
1	X	614	DA	N3-C4-N9	-5.65	122.88	127.40
2	Y	705	DC	C4'-C3'-C2'	5.64	108.18	103.10
2	Y	716	DG	C1'-O4'-C4'	5.63	115.73	110.10
1	X	611	DC	N1-C2-N3	-5.62	115.26	119.20
1	X	623	DA	C3'-C2'-C1'	-5.61	95.77	102.50
2	Y	719	DC	O4'-C1'-N1	-5.60	104.08	108.00
3	B	136	LYS	CD-CE-NZ	5.59	124.56	111.70
1	X	606	DA	O3'-P-O5'	-5.59	93.38	104.00
2	Y	718	DC	O4'-C1'-C2'	5.58	110.36	105.90
1	X	625	DG	O4'-C1'-N9	5.58	111.91	108.00
1	X	604	DT	C5-C6-N1	-5.56	120.36	123.70
1	X	618	DT	N3-C4-C5	5.55	118.53	115.20
2	Y	706	DG	N1-C2-N3	-5.55	120.57	123.90
2	Y	718	DC	C2-N3-C4	-5.55	117.13	119.90
1	X	621	DC	C6-N1-C2	5.54	122.51	120.30
2	Y	721	DT	C6-C5-C7	-5.53	119.58	122.90
3	B	27	VAL	CB-CA-C	-5.53	100.90	111.40
1	X	616	DG	P-O5'-C5'	5.52	129.74	120.90
2	Y	712	DT	N1-C1'-C2'	5.51	123.08	112.60
2	Y	703	DT	O4'-C1'-N1	-5.49	104.16	108.00
2	Y	710	DC	OP1-P-OP2	-5.49	111.37	119.60
2	Y	719	DC	C5-C6-N1	5.48	123.74	121.00
1	X	610	DT	N1-C2-N3	5.47	117.88	114.60
1	X	619	DA	C2-N3-C4	5.47	113.33	110.60
3	A	164	LEU	CB-CG-CD1	5.46	120.28	111.00
1	X	605	DA	P-O3'-C3'	5.45	126.25	119.70
2	Y	726	DG	C8-N9-C4	-5.45	104.22	106.40
2	Y	724	DT	OP1-P-O3'	5.42	117.12	105.20
2	Y	719	DC	C5-C4-N4	5.41	123.99	120.20
1	X	614	DA	C5-C6-N1	-5.41	115.00	117.70
1	X	624	DA	C3'-C2'-C1'	-5.40	96.02	102.50
1	X	626	DC	C6-N1-C2	-5.39	118.14	120.30
3	A	131	GLN	CA-CB-CG	5.37	125.20	113.40
1	X	622	DG	C6-N1-C2	-5.36	121.88	125.10
1	X	614	DA	N3-C4-C5	5.36	130.55	126.80
2	Y	721	DT	N1-C2-O2	-5.35	118.82	123.10
2	Y	705	DC	N1-C1'-C2'	5.33	122.73	112.60
3	A	74	LYS	CD-CE-NZ	-5.33	99.44	111.70
2	Y	721	DT	C6-N1-C2	5.32	123.96	121.30
1	X	618	DT	N3-C4-O4	-5.31	116.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	614	DA	C6-N1-C2	5.31	121.78	118.60
2	Y	720	DG	OP2-P-O3'	5.31	116.88	105.20
2	Y	707	DC	C2-N3-C4	-5.28	117.26	119.90
1	X	625	DG	P-O5'-C5'	-5.28	112.46	120.90
3	B	187	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	X	606	DA	C6-C5-N7	-5.26	128.61	132.30
2	Y	719	DC	OP2-P-O3'	5.24	116.74	105.20
2	Y	726	DG	C4-C5-N7	-5.24	108.70	110.80
1	X	619	DA	C6-N1-C2	5.24	121.74	118.60
1	X	621	DC	O4'-C1'-C2'	-5.24	101.71	105.90
2	Y	723	DA	OP1-P-OP2	5.22	127.43	119.60
2	Y	718	DC	O5'-P-OP2	-5.22	101.00	105.70
2	Y	721	DT	C4'-C3'-C2'	5.18	107.77	103.10
2	Y	723	DA	C5'-C4'-O4'	5.18	119.14	109.30
1	X	608	DG	C8-N9-C4	-5.17	104.33	106.40
2	Y	717	DA	N1-C6-N6	-5.17	115.50	118.60
2	Y	720	DG	N7-C8-N9	-5.17	110.52	113.10
1	X	621	DC	C1'-O4'-C4'	-5.16	104.94	110.10
1	X	613	DT	OP1-P-O3'	5.16	116.55	105.20
2	Y	718	DC	N1-C1'-C2'	5.15	122.39	112.60
1	X	602	DG	P-O3'-C3'	-5.15	113.53	119.70
3	A	134	GLU	OE1-CD-OE2	5.14	129.47	123.30
2	Y	719	DC	OP1-P-OP2	-5.13	111.90	119.60
1	X	602	DG	C8-N9-C4	-5.12	104.35	106.40
1	X	611	DC	N1-C1'-C2'	5.11	122.31	112.60
2	Y	708	DT	O4'-C1'-C2'	-5.10	101.82	105.90
2	Y	718	DC	N3-C2-O2	5.08	125.45	121.90
1	X	615	DA	N1-C6-N6	5.06	121.64	118.60
2	Y	710	DC	C5-C4-N4	-5.06	116.66	120.20
1	X	612	DC	N1-C1'-C2'	5.04	122.18	112.60
2	Y	721	DT	P-O5'-C5'	-5.03	112.85	120.90
2	Y	706	DG	C4-C5-C6	-5.02	115.79	118.80

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	X	535	0	292	20	0
2	Y	525	0	295	30	1
3	A	1669	0	1717	58	0
3	B	1669	0	1717	73	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	X	1	0	0	0	0
5	A	118	0	0	11	0
5	B	78	0	0	11	0
5	X	27	0	0	2	0
5	Y	40	0	0	6	1
All	All	4664	0	4021	166	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (166) 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:B:22:LYS:HD3	5:B:1213:HOH:O	1.40	1.20
2:Y:721:DT:H2"	2:Y:722:DT:H5'	1.21	1.11
3:B:73:THR:HG22	3:B:85:VAL:HG22	1.40	1.01
2:Y:722:DT:O4	5:Y:1236:HOH:O	1.84	0.95
3:B:53:SER:O	3:B:57:LEU:HD22	1.70	0.92
3:B:156:ARG:HH21	3:B:156:ARG:HG2	1.34	0.90
2:Y:721:DT:H2"	2:Y:722:DT:C5'	2.02	0.90
3:B:174:ASP:OD1	3:B:175:LEU:N	2.08	0.86
3:A:94:HIS:HD2	3:A:96:ASN:H	1.16	0.86
3:A:170:ASP:O	3:A:173:GLN:NE2	2.07	0.86
2:Y:721:DT:C2'	2:Y:722:DT:H5'	2.07	0.83
3:A:163:LEU:CD2	3:A:185:ILE:HG21	2.09	0.81
3:A:170:ASP:HB3	3:A:173:GLN:NE2	1.96	0.80
3:A:163:LEU:HD21	3:A:185:ILE:CG2	2.12	0.80
3:B:98:VAL:HG13	3:B:123:LEU:HD12	1.64	0.79
1:X:602:DG:H2"	1:X:603:DA:C8	2.18	0.79
3:B:195:GLN:O	3:B:198:GLU:HG2	1.81	0.79
2:Y:723:DA:H2"	2:Y:724:DT:H5"	1.67	0.77
1:X:606:DA:OP2	5:X:1109:HOH:O	2.02	0.77
3:A:127:ILE:HG22	3:A:133:LEU:HD13	1.66	0.77
3:A:71:ILE:HD12	3:A:189:MET:SD	2.25	0.76
3:A:129:ASN:HD22	3:A:132:SER:H	1.33	0.76
3:A:170:ASP:C	3:A:173:GLN:HE22	1.88	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:163:LEU:HD21	3:A:185:ILE:HG21	1.64	0.75
3:B:197:ASN:H	3:B:197:ASN:HD22	1.34	0.75
3:A:94:HIS:CD2	3:A:96:ASN:H	2.03	0.74
1:X:601:DC:H2"	1:X:602:DG:O5'	1.87	0.74
3:B:166:LEU:HD22	3:B:182:ILE:HG13	1.71	0.72
2:Y:723:DA:H2"	2:Y:724:DT:C5'	2.21	0.71
1:X:612:DC:OP1	5:X:1042:HOH:O	2.08	0.71
3:A:76:LEU:HD22	3:A:78:THR:HG22	1.73	0.71
3:B:201:PRO:HG3	5:B:1115:HOH:O	1.91	0.70
3:A:196:SER:O	5:A:1204:HOH:O	2.08	0.70
3:B:73:THR:CG2	3:B:85:VAL:HG22	2.20	0.70
3:B:156:ARG:HH21	3:B:156:ARG:CG	1.98	0.70
3:A:49:VAL:HG12	3:A:50:GLN:O	1.91	0.69
3:A:76:LEU:CD2	3:A:78:THR:HG22	2.23	0.69
3:B:179:VAL:HA	3:B:183:LEU:HD23	1.75	0.69
2:Y:706:DG:H4'	3:B:28:LYS:HE3	1.74	0.68
3:B:179:VAL:HG23	3:B:207:GLN:HG2	1.74	0.68
3:B:156:ARG:HG2	3:B:156:ARG:NH2	2.08	0.68
1:X:612:DC:N4	2:Y:715:DG:O6	2.19	0.67
3:A:170:ASP:CA	3:A:173:GLN:HE22	2.07	0.67
3:B:174:ASP:CG	3:B:175:LEU:H	1.97	0.67
3:B:179:VAL:CG2	3:B:207:GLN:HG2	2.25	0.66
3:B:175:LEU:O	3:B:179:VAL:HG12	1.96	0.66
3:B:174:ASP:CG	3:B:175:LEU:N	2.49	0.66
3:A:188:GLN:NE2	5:A:1128:HOH:O	2.29	0.65
2:Y:723:DA:C2'	2:Y:724:DT:H5"	2.26	0.65
3:B:156:ARG:CG	3:B:156:ARG:NH2	2.54	0.63
3:B:20:LEU:HD11	3:B:114:ARG:HA	1.80	0.62
3:B:76:LEU:HB3	3:B:79:SER:OG	2.00	0.61
3:B:192:GLN:HE21	3:B:195:GLN:NE2	1.99	0.61
3:A:129:ASN:ND2	3:A:132:SER:H	2.00	0.60
3:B:127:ILE:HG22	3:B:133:LEU:HD13	1.83	0.60
3:A:12:LEU:HD22	3:A:13:PRO:HD2	1.83	0.60
3:B:98:VAL:HG13	3:B:123:LEU:CD1	2.32	0.59
3:B:204:GLU:HA	3:B:207:GLN:HB2	1.84	0.59
1:X:612:DC:N3	2:Y:715:DG:N1	2.42	0.59
3:A:179:VAL:HG13	3:A:207:GLN:HG2	1.86	0.58
2:Y:709:DA:H1'	2:Y:710:DC:H5"	1.85	0.57
1:X:621:DC:H2"	1:X:622:DG:C8	2.39	0.57
3:B:6:LEU:HD13	3:B:10:GLU:HG2	1.86	0.56
3:B:105:LEU:HD13	3:B:125:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:95:VAL:O	3:B:98:VAL:HG22	2.05	0.56
3:A:143:GLN:NE2	3:A:144:TYR:CZ	2.73	0.56
3:A:166:LEU:HD22	5:A:1091:HOH:O	2.05	0.56
1:X:616:DG:O6	3:B:116:LYS:CE	2.54	0.55
1:X:602:DG:H2"	1:X:603:DA:H8	1.70	0.55
1:X:614:DA:C8	1:X:614:DA:H5"	2.41	0.55
2:Y:703:DT:H5"	3:B:173:GLN:HE22	1.72	0.55
1:X:602:DG:H4'	1:X:602:DG:OP1	2.07	0.55
3:A:94:HIS:HD2	3:A:96:ASN:N	1.95	0.54
3:B:188:GLN:HG3	5:B:1158:HOH:O	2.07	0.54
3:B:95:VAL:CG2	3:B:121:ALA:HB1	2.37	0.54
5:A:1166:HOH:O	3:B:49:VAL:HG21	2.08	0.54
2:Y:712:DT:H4'	3:B:192:GLN:HG2	1.89	0.54
2:Y:722:DT:C7	5:Y:1236:HOH:O	2.55	0.53
2:Y:723:DA:H1'	2:Y:724:DT:H5"	1.89	0.53
3:A:90:ASN:ND2	5:A:1032:HOH:O	2.41	0.53
2:Y:722:DT:H71	5:Y:1236:HOH:O	2.07	0.53
3:A:28:LYS:O	3:A:31:LYS:HE2	2.09	0.53
3:A:161:LYS:O	3:A:165:GLU:HG3	2.09	0.53
3:B:59:LEU:HD13	3:B:103:LEU:HD13	1.91	0.53
3:A:170:ASP:CB	3:A:173:GLN:NE2	2.71	0.52
2:Y:705:DC:H2"	2:Y:706:DG:O5'	2.09	0.52
3:A:170:ASP:HB3	3:A:173:GLN:CD	2.29	0.52
1:X:625:DG:H2"	1:X:626:DC:C5	2.44	0.52
3:A:18:GLU:HG3	5:A:1181:HOH:O	2.09	0.52
2:Y:711:DC:H3'	5:Y:1074:HOH:O	2.10	0.51
3:A:163:LEU:HD22	3:A:185:ILE:HG21	1.92	0.51
3:A:75:LYS:CE	5:A:1136:HOH:O	2.58	0.51
3:B:116:LYS:HG3	5:B:1225:HOH:O	2.11	0.51
3:A:170:ASP:HB3	3:A:173:GLN:HE22	1.72	0.51
2:Y:709:DA:H2"	2:Y:710:DC:H5'	1.92	0.51
3:A:170:ASP:O	3:A:173:GLN:CD	2.49	0.51
3:A:170:ASP:CB	3:A:173:GLN:HE22	2.24	0.50
3:B:81:PHE:CE2	3:B:175:LEU:HD23	2.46	0.50
3:B:172:HIS:CD2	3:B:172:HIS:H	2.27	0.50
3:B:105:LEU:HD13	3:B:125:LEU:CD1	2.41	0.50
3:A:163:LEU:HD21	3:A:185:ILE:HG22	1.94	0.50
1:X:619:DA:C2	2:Y:709:DA:C2	2.99	0.50
3:A:57:LEU:HD13	3:A:144:TYR:HD2	1.75	0.50
2:Y:703:DT:OP1	3:B:80:LYS:HB2	2.12	0.49
3:B:156:ARG:NH2	5:B:1135:HOH:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:71:ILE:CD1	3:A:189:MET:SD	3.00	0.49
3:B:62:PHE:HZ	3:B:93:ARG:HD3	1.78	0.49
3:B:95:VAL:HG23	3:B:121:ALA:HB1	1.95	0.49
1:X:618:DT:H4'	3:B:195:GLN:HE22	1.78	0.49
3:B:22:LYS:NZ	5:B:1213:HOH:O	2.43	0.48
3:B:202:ASN:ND2	3:B:205:ALA:H	2.10	0.48
3:B:171:ALA:HB1	3:B:177:GLN:HB3	1.96	0.48
3:A:23:ILE:HD12	3:A:43:LEU:HD22	1.96	0.47
3:A:108:PHE:O	3:A:136:LYS:HE3	2.14	0.47
3:B:14:GLN:HA	3:B:17:LEU:HD12	1.96	0.47
3:A:127:ILE:CG2	3:A:133:LEU:HD13	2.42	0.47
3:A:106:GLU:OE1	3:A:109:LYS:NZ	2.47	0.47
3:B:122:THR:CG2	5:B:1010:HOH:O	2.63	0.47
3:A:75:LYS:HE2	5:A:1136:HOH:O	2.13	0.47
3:A:93:ARG:NH2	5:A:1051:HOH:O	2.22	0.47
3:A:146:VAL:HG13	3:A:154:VAL:HG22	1.96	0.47
2:Y:718:DC:C2'	2:Y:719:DC:H5'	2.45	0.46
3:A:77:ALA:HA	5:A:1066:HOH:O	2.14	0.46
3:B:167:PHE:HD1	3:B:172:HIS:CD2	2.33	0.46
2:Y:703:DT:OP1	3:B:173:GLN:OE1	2.34	0.46
3:A:28:LYS:NZ	5:A:1106:HOH:O	2.49	0.46
3:A:47:ASP:O	3:A:49:VAL:HG23	2.16	0.46
3:B:166:LEU:HD23	3:B:171:ALA:CB	2.45	0.46
1:X:614:DA:H2'	1:X:614:DA:H5'	1.42	0.45
2:Y:704:DT:H3'	5:Y:1151:HOH:O	2.14	0.45
1:X:601:DC:C2'	1:X:602:DG:O5'	2.61	0.45
3:A:23:ILE:HG12	3:A:39:ASP:HB3	1.99	0.45
3:A:180:ASN:O	3:A:184:PRO:HG2	2.17	0.45
3:B:188:GLN:HG3	3:B:188:GLN:O	2.16	0.45
3:B:188:GLN:CG	5:B:1158:HOH:O	2.65	0.45
3:B:7:LYS:O	3:B:10:GLU:HB3	2.17	0.44
2:Y:723:DA:H2"	2:Y:724:DT:H5'	1.98	0.44
1:X:617:DG:H1'	1:X:618:DT:H5"	1.99	0.44
2:Y:723:DA:C1'	2:Y:724:DT:H5"	2.47	0.44
2:Y:706:DG:H5"	3:B:28:LYS:HG3	1.99	0.44
3:B:57:LEU:HD13	3:B:144:TYR:HD2	1.82	0.44
2:Y:721:DT:H2'	2:Y:722:DT:C6	2.53	0.44
3:B:155:LYS:HE3	3:B:188:GLN:OE1	2.18	0.43
5:Y:1187:HOH:O	3:A:153:LYS:HE3	2.17	0.43
3:B:6:LEU:CD1	3:B:10:GLU:O	2.66	0.43
3:B:153:LYS:HG2	5:B:1127:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:ASN:HD22	3:A:197:ASN:H	1.66	0.43
1:X:616:DG:O6	3:B:116:LYS:HE3	2.18	0.43
3:B:22:LYS:CD	5:B:1213:HOH:O	2.23	0.43
3:B:90:ASN:HA	3:B:125:LEU:O	2.17	0.43
3:A:146:VAL:O	3:A:146:VAL:CG1	2.66	0.43
3:A:61:GLY:HA3	3:B:58:PHE:O	2.19	0.42
3:A:177:GLN:HE21	3:A:181:LYS:HD2	1.84	0.42
3:B:122:THR:HG22	5:B:1010:HOH:O	2.18	0.42
3:B:179:VAL:HG22	3:B:207:GLN:HG2	1.99	0.41
1:X:608:DG:H2"	1:X:609:DG:O5'	2.20	0.41
3:A:171:ALA:HB1	3:A:177:GLN:HB3	2.03	0.41
1:X:611:DC:H5'	3:A:197:ASN:HB3	2.02	0.41
3:B:82:GLY:HA3	3:B:209:PHE:HE2	1.86	0.41
2:Y:720:DG:H2"	2:Y:721:DT:O5'	2.21	0.41
3:B:73:THR:HG23	3:B:186:TRP:CD1	2.56	0.41
3:B:145:VAL:HG12	3:B:149:SER:HB2	2.03	0.41
2:Y:716:DG:O6	3:A:116:LYS:CE	2.69	0.40
3:A:168:ASN:HD22	3:A:168:ASN:HA	1.53	0.40
3:B:174:ASP:OD1	3:B:174:ASP:C	2.60	0.40
3:B:209:PHE:C	3:B:211:ARG:H	2.24	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:701:DG:O5'	5:Y:1234:HOH:O[2_674]	1.80	0.40

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
3	A	205/207 (99%)	198 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	B	205/207 (99%)	185 (90%)	16 (8%)	4 (2%)	7 4
All	All	410/414 (99%)	383 (93%)	23 (6%)	4 (1%)	15 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	204	GLU
3	B	203	LEU
3	B	96	ASN
3	B	184	PRO

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
3	A	185/185 (100%)	159 (86%)	26 (14%)	3 2
3	B	185/185 (100%)	161 (87%)	24 (13%)	4 3
All	All	370/370 (100%)	320 (86%)	50 (14%)	4 3

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	15	ASP
3	A	47	ASP
3	A	48	GLU
3	A	50	GLN
3	A	54	GLU
3	A	57	LEU
3	A	70	ASN
3	A	83	LEU
3	A	90	ASN
3	A	101	LEU
3	A	103	LEU

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Mol	Chain	Res	Type
3	A	107	VAL
3	A	122	THR
3	A	123	LEU
3	A	125	LEU
3	A	133	LEU
3	A	139	PRO
3	A	143	GLN
3	A	153	LYS
3	A	164	LEU
3	A	173	GLN
3	A	175	LEU
3	A	183	LEU
3	A	191	LYS
3	A	197	ASN
3	B	7	LYS
3	B	14	GLN
3	B	20	LEU
3	B	27	VAL
3	B	31	LYS
3	B	45	GLN
3	B	57	LEU
3	B	70	ASN
3	B	90	ASN
3	B	95	VAL
3	B	98	VAL
3	B	101	LEU
3	B	103	LEU
3	B	105	LEU
3	B	106	GLU
3	B	122	THR
3	B	124	VAL
3	B	133	LEU
3	B	156	ARG
3	B	164	LEU
3	B	166	LEU
3	B	174	ASP
3	B	196	SER
3	B	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	50	GLN
3	A	70	ASN
3	A	90	ASN
3	A	94	HIS
3	A	129	ASN
3	A	159	ASN
3	A	168	ASN
3	A	173	GLN
3	A	177	GLN
3	A	192	GLN
3	A	193	GLN
3	A	197	ASN
3	B	14	GLN
3	B	159	ASN
3	B	168	ASN
3	B	172	HIS
3	B	173	GLN
3	B	180	ASN
3	B	195	GLN
3	B	197	ASN
3	B	202	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 3 ligands modelled in this entry, 3 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	X	26/26 (100%)	-0.15	0	100	100	38, 48, 71, 86	0
2	Y	26/26 (100%)	-0.14	1 (3%)	40	38	28, 49, 61, 62	0
3	A	207/207 (100%)	-0.29	4 (1%)	66	65	21, 34, 53, 62	0
3	B	207/207 (100%)	0.05	4 (1%)	66	65	20, 44, 72, 77	0
All	All	466/466 (100%)	-0.12	9 (1%)	66	65	20, 40, 66, 86	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	49	VAL	2.6
3	A	173	GLN	2.4
3	B	50	GLN	2.4
3	B	204	GLU	2.3
3	A	48	GLU	2.2
3	B	14	GLN	2.2
3	A	77	ALA	2.1
3	B	73	THR	2.1
2	Y	726	DG	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
4	CA	B	803	1/1	0.96	0.13	51,51,51,51	0
4	CA	X	802	1/1	0.98	0.06	36,36,36,36	0
4	CA	A	801	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.