W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:01 PM GMT

|		
PDB ID	:	4UMK
Title	:	The complex of Spo0J and parS DNA in chromosomal partition system
Authors	:	Chen, B.W.; Chu, C.H.; Tung, J.Y.; Hsu, C.E.; Hsiao, C.D.; Sun, Y.J.
Deposited on	:	2014-05-19
Resolution	:	3.10 Å(reported)

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
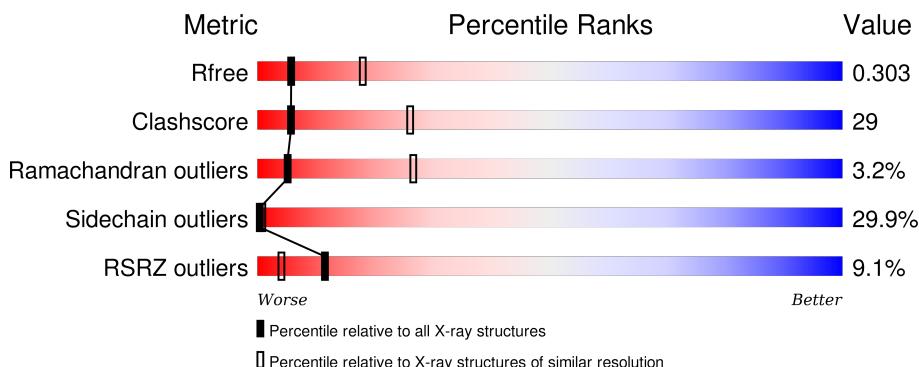
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	240	3% 29% 30% 11% • 28%
1	B	240	8% 28% 35% 12% • 24%
1	C	240	10% 37% 28% 15% 20%
1	D	240	10% 33% 26% 13% • 27%
2	W	24	25% 33% 42%

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Mol	Chain	Length	Quality of chain
2	Z	24	29% 38% 33%
3	X	24	8% 33% 58%
3	Y	24	8% 42% 50%
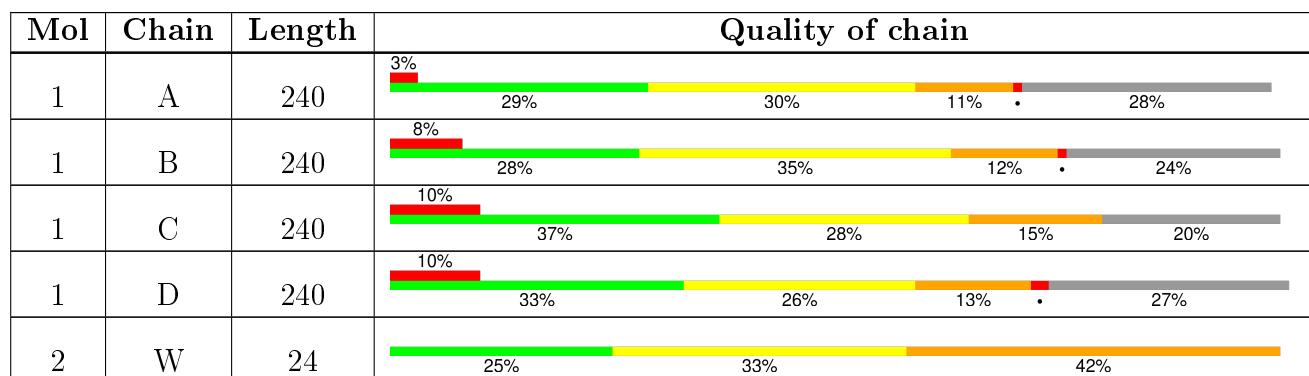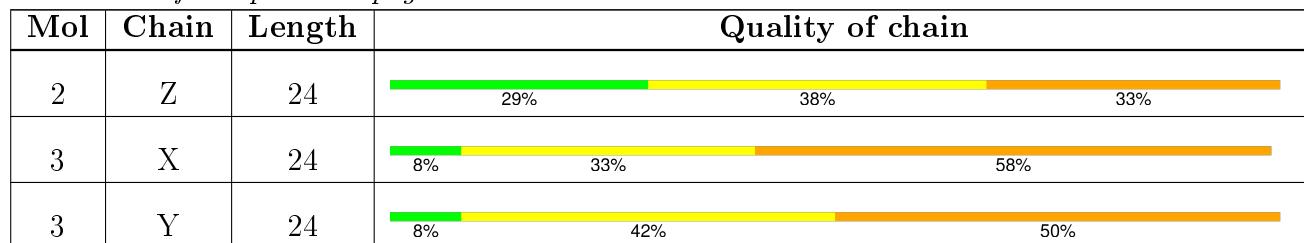
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	1228	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7994 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 PROBABLE CHROMOSOME-PARTITIONING PROTEIN PARB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1367	858	244	261	4			
1	B	183	Total	C	N	O	S	0	0	0
			1463	920	261	278	4			
1	C	193	Total	C	N	O	S	0	0	0
			1535	964	271	295	5			
1	D	176	Total	C	N	O	S	0	0	0
			1400	880	248	268	4			

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	24	Total	C	N	O	P	0	0	0
			501	236	100	141	24			
2	Z	24	Total	C	N	O	P	0	0	0
			501	236	100	141	24			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	24	Total	C	N	O	P	0	0	0
			483	231	81	147	24			
3	Y	24	Total	C	N	O	P	0	0	0
			483	231	81	147	24			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
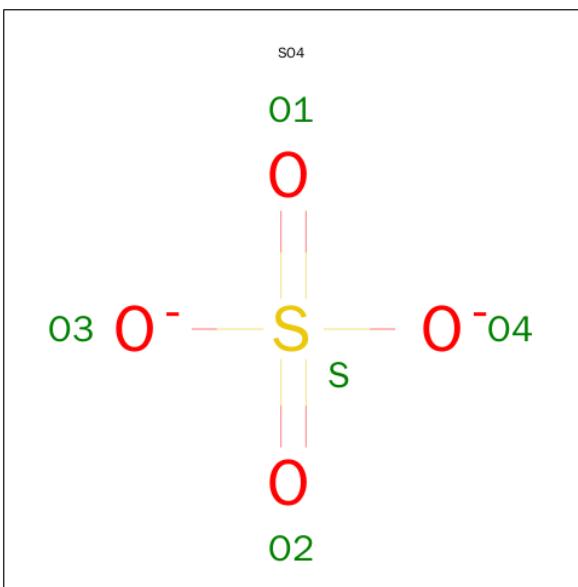
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	W	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	47	Total 47	O 47	0	0
5	C	45	Total 45	O 45	0	0
5	D	31	Total 31	O 31	0	0
5	W	16	Total 16	O 16	0	0
5	X	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Y	16	Total 16	O 16	0	0
5	Z	16	Total 16	O 16	0	0

3 Residue-property plots (i)

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

- Molecule 1: PROBABLE CHROMOSOME-PARTITIONING PROTEIN PARB
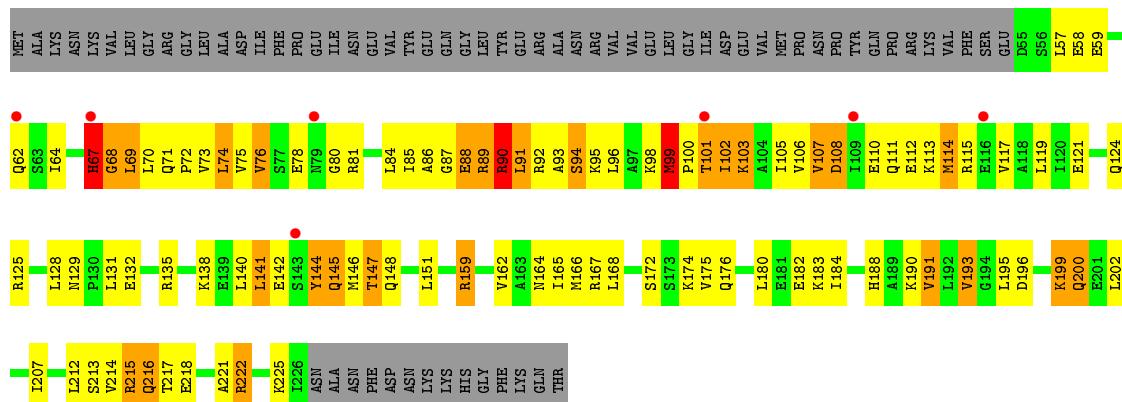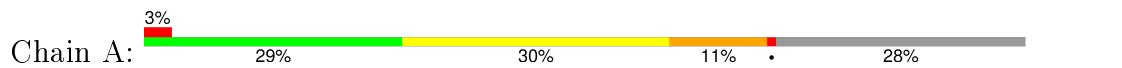
- Molecule 1: PROBABLE CHROMOSOME-PARTITIONING PROTEIN PARB

- Molecule 1: PROBABLE CHROMOSOME-PARTITIONING PROTEIN PARB

• Molecule 1: PROBABLE CHROMOSOME-PARTITIONING PROTEIN PARB

Chain D:

• Molecule 2: DNA

Chain W:

• Molecule 2: DNA

Chain Z:

• Molecule 3: DNA

Chain X:

• Molecule 3: DNA

Chain Y:
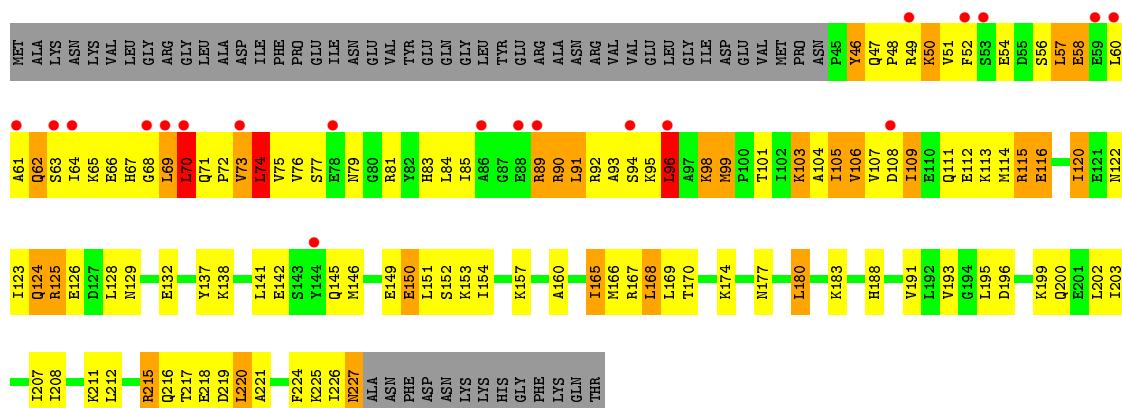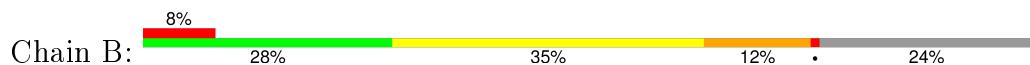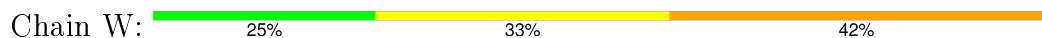
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.48Å 232.73Å 78.34Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	23.57 – 3.10 23.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (23.57-3.10) 91.4 (23.57-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.37 (at 3.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.251 , 0.299 0.254 , 0.303	Depositor DCC
R_{free} test set	1926 reflections (5.99%)	DCC
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.0	EDS
Estimated twinning fraction	0.119 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	1 of 33299 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7994	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.51	0/1377	0.79	2/1847 (0.1%)
1	B	0.47	0/1477	0.78	2/1982 (0.1%)
1	C	0.51	0/1550	0.76	1/2084 (0.0%)
1	D	0.52	1/1411 (0.1%)	0.75	0/1893
2	W	1.14	1/564 (0.2%)	2.16	28/870 (3.2%)
2	Z	1.25	3/564 (0.5%)	2.36	39/870 (4.5%)
3	X	1.29	3/538 (0.6%)	2.46	46/826 (5.6%)
3	Y	1.32	6/538 (1.1%)	2.44	45/826 (5.4%)
All	All	0.78	14/8019 (0.2%)	1.45	163/11198 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	3
All	All	0	5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	7	DT	C1'-N1	7.49	1.58	1.49
3	Y	7	DT	N1-C2	6.56	1.43	1.38
3	Y	1	DT	C2-O2	6.14	1.27	1.22
2	Z	5	DT	C1'-N1	6.02	1.57	1.49
3	X	1	DT	N1-C2	6.00	1.42	1.38
3	X	8	DT	C3'-O3'	-5.93	1.36	1.44
2	W	12	DC	C3'-O3'	-5.93	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	1	DT	C1'-N1	5.84	1.56	1.49
3	Y	15	DG	C3'-O3'	-5.84	1.36	1.44
3	Y	1	DT	C2-N3	5.70	1.42	1.37
2	Z	4	DG	P-O5'	5.69	1.65	1.59
3	X	13	DG	C3'-O3'	-5.04	1.37	1.44
1	D	102	ILE	CA-CB	5.03	1.66	1.54
2	Z	14	DT	C3'-O3'	-5.01	1.37	1.44

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	13	DG	O4'-C1'-N9	-15.45	97.19	108.00
2	Z	1	DA	N1-C6-N6	-14.39	109.97	118.60
2	W	14	DT	O4'-C1'-N1	-14.33	97.97	108.00
2	Z	7	DT	N3-C4-O4	12.71	127.52	119.90
2	Z	1	DA	C5-C6-N6	12.37	133.60	123.70
3	X	13	DG	O4'-C1'-N9	-12.33	99.37	108.00
2	Z	7	DT	O4'-C1'-N1	-12.20	99.46	108.00
2	W	8	DT	N3-C4-O4	11.78	126.97	119.90
3	Y	4	DC	O4'-C1'-C2'	-11.56	96.65	105.90
3	Y	1	DT	N3-C4-O4	11.50	126.80	119.90
3	Y	8	DT	N3-C4-O4	11.11	126.57	119.90
2	W	7	DT	C5-C4-O4	-10.81	117.33	124.90
3	Y	9	DT	N3-C4-O4	10.68	126.31	119.90
3	X	14	DT	N3-C2-O2	-10.46	116.03	122.30
2	Z	1	DA	N9-C4-C5	10.38	109.95	105.80
3	Y	14	DT	O4'-C4'-C3'	-10.35	99.79	106.00
3	X	24	DT	O4'-C1'-N1	-10.34	100.76	108.00
3	Y	7	DT	N3-C2-O2	-10.33	116.10	122.30
2	Z	7	DT	C5-C4-O4	-10.13	117.81	124.90
3	Y	9	DT	C5-C4-O4	-9.98	117.91	124.90
2	W	8	DT	C5-C4-O4	-9.96	117.93	124.90
2	Z	5	DT	O4'-C1'-N1	9.95	114.97	108.00
3	X	7	DT	N3-C4-O4	9.94	125.86	119.90
3	X	12	DC	O4'-C4'-C3'	-9.78	100.14	106.00
2	W	7	DT	N3-C4-O4	9.45	125.57	119.90
2	W	20	DA	O4'-C1'-N9	9.41	114.59	108.00
2	Z	1	DA	O4'-C4'-C3'	-9.30	100.42	106.00
2	W	7	DT	C6-C5-C7	9.21	128.43	122.90
3	X	9	DT	O4'-C1'-N1	-9.08	101.64	108.00
3	X	5	DT	N3-C4-O4	9.07	125.34	119.90
2	W	14	DT	O4'-C4'-C3'	-8.98	100.61	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	10	DC	O4'-C4'-C3'	-8.91	100.65	106.00
2	Z	14	DT	O5'-P-OP2	-8.53	98.02	105.70
3	Y	23	DC	O4'-C1'-N1	8.53	113.97	108.00
3	X	17	DA	O4'-C1'-N9	-8.52	102.04	108.00
3	X	24	DT	N1-C2-O2	-8.46	116.33	123.10
3	X	5	DT	C5-C4-O4	-8.43	119.00	124.90
3	Y	7	DT	C6-N1-C2	-8.36	117.12	121.30
2	W	7	DT	C4-C5-C7	-8.35	113.99	119.00
2	Z	14	DT	O4'-C1'-N1	-8.34	102.17	108.00
2	W	13	DG	O4'-C1'-N9	-8.29	102.20	108.00
3	Y	16	DG	O4'-C4'-C3'	-8.13	101.12	106.00
3	Y	6	DG	O4'-C1'-N9	8.11	113.68	108.00
3	X	24	DT	O5'-C5'-C4'	-8.08	90.80	111.00
3	X	21	DC	O4'-C1'-N1	8.05	113.63	108.00
2	Z	1	DA	C4-C5-N7	-8.05	106.68	110.70
2	Z	1	DA	C6-C5-N7	8.02	137.91	132.30
3	Y	10	DC	O4'-C1'-C2'	-8.00	99.50	105.90
1	B	74	LEU	CA-CB-CG	7.82	133.28	115.30
3	Y	8	DT	C5-C4-O4	-7.58	119.59	124.90
3	X	24	DT	N3-C2-O2	7.58	126.85	122.30
2	Z	14	DT	N3-C2-O2	-7.56	117.76	122.30
3	X	23	DC	O4'-C4'-C3'	-7.53	101.48	106.00
2	Z	1	DA	N3-C4-N9	-7.52	121.39	127.40
3	X	1	DT	C5-C4-O4	-7.46	119.67	124.90
3	Y	14	DT	N3-C4-O4	7.44	124.36	119.90
3	Y	5	DT	N3-C4-O4	7.40	124.34	119.90
3	X	7	DT	C5-C4-O4	-7.37	119.74	124.90
3	X	24	DT	C2-N3-C4	-7.32	122.81	127.20
3	Y	21	DC	O4'-C4'-C3'	-7.29	101.58	104.50
2	Z	6	DG	O4'-C4'-C3'	-7.27	101.59	104.50
3	X	24	DT	C6-C5-C7	-7.26	118.54	122.90
2	Z	6	DG	C6-C5-N7	-7.23	126.06	130.40
2	Z	7	DT	P-O5'-C5'	-7.23	109.33	120.90
3	X	16	DG	O4'-C1'-N9	7.15	113.00	108.00
3	Y	4	DC	O4'-C1'-N1	7.14	113.00	108.00
2	W	8	DT	P-O5'-C5'	-7.13	109.49	120.90
3	X	1	DT	N3-C2-O2	-7.10	118.04	122.30
3	X	12	DC	O4'-C1'-N1	-7.04	103.07	108.00
3	Y	6	DG	N3-C4-C5	-7.03	125.08	128.60
1	B	96	LEU	CA-CB-CG	7.00	131.40	115.30
3	X	1	DT	N3-C4-O4	6.98	124.09	119.90
3	Y	7	DT	O4'-C1'-N1	6.95	112.87	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	7	DT	N1-C2-O2	6.93	128.65	123.10
3	Y	1	DT	O4'-C1'-N1	6.92	112.85	108.00
2	W	14	DT	N1-C1'-C2'	6.85	125.61	112.60
3	Y	9	DT	C4-C5-C7	-6.83	114.90	119.00
2	Z	13	DG	O4'-C1'-C2'	-6.79	100.47	105.90
3	X	24	DT	C5-C4-O4	-6.77	120.16	124.90
2	Z	8	DT	N3-C4-O4	6.77	123.96	119.90
2	W	22	DG	O4'-C1'-N9	6.75	112.72	108.00
3	Y	8	DT	N3-C2-O2	-6.74	118.25	122.30
2	Z	6	DG	C4'-C3'-C2'	-6.71	97.06	103.10
3	X	14	DT	O4'-C1'-N1	-6.70	103.31	108.00
3	X	15	DG	O4'-C1'-N9	6.56	112.59	108.00
3	Y	6	DG	N3-C4-N9	6.49	129.89	126.00
2	Z	5	DT	N1-C2-N3	6.43	118.46	114.60
3	Y	4	DC	C2-N1-C1'	6.42	125.86	118.80
2	W	8	DT	C4-C5-C7	-6.42	115.15	119.00
3	Y	9	DT	N3-C2-O2	-6.41	118.46	122.30
3	Y	11	DA	O4'-C1'-N9	6.37	112.46	108.00
2	Z	9	DC	O4'-C1'-N1	6.35	112.44	108.00
3	Y	18	DA	O4'-C1'-N9	6.29	112.41	108.00
3	X	13	DG	C6-C5-N7	-6.26	126.64	130.40
3	Y	16	DG	C4'-C3'-C2'	-6.23	97.50	103.10
3	X	13	DG	O4'-C4'-C3'	-6.19	102.02	104.50
3	Y	2	DC	O4'-C1'-N1	-6.17	103.68	108.00
1	C	57	LEU	CA-CB-CG	6.11	129.35	115.30
2	Z	9	DC	C4'-C3'-C2'	-6.09	97.62	103.10
3	Y	14	DT	N3-C2-O2	-6.09	118.65	122.30
3	X	22	DC	C2-N1-C1'	6.05	125.46	118.80
3	Y	1	DT	C5-C4-O4	-6.02	120.69	124.90
3	Y	5	DT	O4'-C1'-N1	6.02	112.21	108.00
2	Z	6	DG	N1-C6-O6	6.01	123.50	119.90
3	Y	21	DC	C1'-O4'-C4'	-5.96	104.14	110.10
3	X	24	DT	C5'-C4'-C3'	5.95	124.81	114.10
2	Z	15	DG	C3'-C2'-C1'	-5.89	95.43	102.50
3	X	24	DT	N3-C4-O4	5.85	123.41	119.90
3	Y	14	DT	C5-C4-O4	-5.85	120.81	124.90
3	X	11	DA	O4'-C1'-N9	5.84	112.09	108.00
3	X	14	DT	N1-C2-O2	5.82	127.75	123.10
2	W	4	DG	C4'-C3'-C2'	5.81	108.33	103.10
2	Z	14	DT	N3-C4-O4	5.79	123.37	119.90
2	W	24	DA	N1-C6-N6	5.73	122.04	118.60
3	X	8	DT	N3-C4-O4	5.73	123.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	15	DG	C8-N9-C4	-5.72	104.11	106.40
3	X	10	DC	C3'-C2'-C1'	-5.72	95.64	102.50
3	Y	15	DG	O4'-C1'-C2'	-5.71	101.33	105.90
2	Z	7	DT	O4'-C1'-C2'	-5.68	101.36	105.90
3	Y	19	DC	C1'-O4'-C4'	-5.67	104.43	110.10
3	Y	7	DT	N3-C4-O4	5.66	123.30	119.90
3	X	7	DT	C4-C5-C7	-5.65	115.61	119.00
2	W	21	DG	C4'-C3'-C2'	-5.59	98.07	103.10
2	W	8	DT	C6-C5-C7	5.50	126.20	122.90
2	W	16	DA	O4'-C1'-N9	5.47	111.83	108.00
2	Z	1	DA	N1-C2-N3	5.46	132.03	129.30
3	Y	6	DG	C6-C5-N7	-5.46	127.12	130.40
3	Y	10	DC	C3'-C2'-C1'	-5.44	95.97	102.50
3	Y	10	DC	C1'-O4'-C4'	-5.42	104.68	110.10
3	Y	5	DT	P-O5'-C5'	-5.41	112.24	120.90
1	A	90	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	X	13	DG	C5-C6-O6	-5.40	125.36	128.60
2	Z	5	DT	N3-C2-O2	-5.38	119.07	122.30
2	W	12	DC	O4'-C1'-N1	5.37	111.76	108.00
3	X	24	DT	C5-C6-N1	-5.35	120.49	123.70
1	A	99	MET	CA-CB-CG	5.33	122.36	113.30
3	Y	5	DT	C5'-C4'-C3'	-5.33	104.50	114.10
2	W	15	DG	O4'-C1'-N9	-5.33	104.27	108.00
2	W	13	DG	C1'-O4'-C4'	5.32	115.42	110.10
2	Z	5	DT	O4'-C4'-C3'	5.27	109.16	106.00
3	X	14	DT	C6-N1-C2	-5.26	118.67	121.30
3	X	1	DT	N1-C1'-C2'	5.25	122.58	112.60
2	W	24	DA	C4'-C3'-C2'	-5.24	98.38	103.10
2	Z	16	DA	P-O5'-C5'	-5.22	112.55	120.90
2	W	11	DA	N1-C6-N6	5.20	121.72	118.60
3	X	13	DG	N3-C4-N9	5.19	129.11	126.00
2	W	14	DT	O4'-C1'-C2'	-5.18	101.75	105.90
2	Z	8	DT	C5-C4-O4	-5.16	121.29	124.90
2	W	4	DG	N1-C6-O6	5.16	122.99	119.90
2	Z	14	DT	C5-C4-O4	-5.12	121.32	124.90
3	X	22	DC	C6-N1-C2	-5.12	118.25	120.30
2	Z	13	DG	N3-C4-N9	5.11	129.07	126.00
2	W	21	DG	N3-C4-C5	5.09	131.15	128.60
3	Y	9	DT	O4'-C1'-N1	-5.09	104.44	108.00
2	Z	5	DT	N3-C4-O4	5.09	122.95	119.90
2	W	16	DA	C3'-C2'-C1'	-5.08	96.40	102.50
3	X	22	DC	N1-C2-O2	5.08	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	1	DT	O4'-C1'-C2'	5.07	109.96	105.90
2	Z	6	DG	C5-C6-O6	-5.07	125.56	128.60
2	Z	9	DC	N3-C4-N4	-5.06	114.46	118.00
3	X	10	DC	C4'-C3'-C2'	-5.05	98.55	103.10
3	X	1	DT	N1-C2-O2	5.05	127.14	123.10
2	Z	13	DG	N3-C4-C5	-5.02	126.09	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	HIS	Peptide
1	B	74	LEU	Peptide
1	D	101	THR	Peptide
1	D	77	SER	Peptide
1	D	81	ARG	Peptide

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	1367	0	1447	124	0
1	B	1463	0	1540	108	0
1	C	1535	0	1600	73	0
1	D	1400	0	1476	76	0
2	W	501	0	269	30	0
2	Z	501	0	269	23	0
3	X	483	0	272	21	0
3	Y	483	0	272	27	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	W	5	0	0	0	0
5	A	53	0	0	5	0
5	B	47	0	0	9	0
5	C	45	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	31	0	0	4	0
5	W	16	0	0	3	0
5	X	7	0	0	1	0
5	Y	16	0	0	1	0
5	Z	16	0	0	2	0
All	All	7994	0	7145	429	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 29.

All (429) 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:24:DT:H4'	3:Y:24:DT:OP1	1.49	1.10
2:Z:4:DG:H2"	2:Z:5:DT:H5"	1.36	1.07
2:W:3:DG:H1	3:X:22:DC:H42	1.02	1.00
2:W:3:DG:H1	3:X:22:DC:N4	1.68	0.91
1:A:102:ILE:HD12	1:A:106:VAL:HG11	1.53	0.90
1:D:123:ILE:HD11	1:D:155:VAL:HG12	1.55	0.88
1:B:74:LEU:H	1:B:90:ARG:HH21	1.24	0.86
1:B:62:GLN:HA	1:B:65:LYS:HG2	1.59	0.85
1:A:75:VAL:HG12	1:A:84:LEU:HA	1.59	0.84
1:A:67:HIS:HB2	1:A:70:LEU:HA	1.60	0.84
1:C:42:MET:HG2	1:C:145:GLN:HB2	1.60	0.83
2:W:20:DA:H61	3:X:5:DT:H3	1.27	0.82
1:C:60:LEU:HG	1:C:62:GLN:HB3	1.63	0.79
1:A:89:ARG:HH21	1:B:89:ARG:HE	1.30	0.78
1:C:119:LEU:HD21	1:C:139:GLU:HB3	1.64	0.77
1:A:148:GLN:NE2	2:W:5:DT:H3'	1.99	0.77
1:B:51:VAL:HG12	1:B:91:LEU:HD11	1.66	0.76
2:W:21:DG:H1	3:X:4:DC:H42	1.34	0.75
1:D:140:LEU:HA	1:D:144:TYR:CE1	2.22	0.74
1:B:74:LEU:O	1:B:90:ARG:NE	2.20	0.74
1:A:159:ARG:HH21	2:W:5:DT:H2'	1.53	0.74
1:A:69:LEU:HD22	1:A:69:LEU:H	1.53	0.73
1:C:42:MET:O	1:C:145:GLN:NE2	2.22	0.73
1:B:79:ASN:HB2	1:B:111:GLN:HB2	1.69	0.73
2:W:20:DA:N6	3:X:5:DT:H3	1.86	0.73
1:D:103:LYS:HD2	1:D:105:ILE:HG23	1.71	0.73
1:A:74:LEU:HD22	1:A:85:ILE:HD12	1.70	0.72
2:W:23:DG:N7	5:W:2014:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLU:O	1:D:80:GLY:N	2.22	0.72
1:D:65:LYS:O	1:D:65:LYS:NZ	2.23	0.72
1:D:103:LYS:HE2	1:D:106:VAL:HG13	1.71	0.71
1:D:78:GLU:OE1	1:D:78:GLU:N	2.24	0.70
1:A:78:GLU:HB3	1:A:81:ARG:H	1.54	0.70
3:Y:3:DC:H42	2:Z:22:DG:H1	1.38	0.70
1:C:149:GLU:OE1	1:C:150:GLU:N	2.25	0.70
1:C:53:SER:OG	1:C:90:ARG:NH2	2.23	0.69
1:B:85:ILE:HD11	1:B:90:ARG:HB3	1.74	0.69
1:B:74:LEU:HD13	1:B:90:ARG:CZ	2.22	0.69
1:D:140:LEU:HA	1:D:144:TYR:HE1	1.55	0.69
1:C:70:LEU:HD22	1:C:71:GLN:H	1.58	0.69
1:D:78:GLU:HG2	1:D:101:THR:HB	1.74	0.69
1:D:75:VAL:HG11	1:D:95:LYS:HE2	1.75	0.68
5:Y:2004:HOH:O	2:Z:23:DG:N2	2.26	0.68
1:D:196:ASP:N	1:D:196:ASP:OD1	2.25	0.68
1:A:103:LYS:NZ	5:A:2021:HOH:O	2.27	0.68
1:A:164:ASN:HA	1:A:167:ARG:HD3	1.75	0.67
2:Z:22:DG:H2'	2:Z:23:DG:C8	2.29	0.67
1:A:100:PRO:HD2	1:A:101:THR:H	1.60	0.66
1:C:73:VAL:HG22	1:C:108:ASP:HB3	1.76	0.66
1:A:191:VAL:HG11	1:A:217:THR:HG22	1.77	0.66
1:A:62:GLN:HE22	1:A:90:ARG:HA	1.60	0.66
1:C:112:GLU:OE1	1:C:115:ARG:NH1	2.29	0.65
2:W:21:DG:H1	3:X:4:DC:N4	1.93	0.65
1:A:114:MET:HG3	1:C:89:ARG:HH21	1.62	0.65
1:A:67:HIS:CD2	1:A:68:GLY:O	2.48	0.65
3:Y:14:DT:H2"	3:Y:15:DG:O5'	1.97	0.65
1:B:124:GLN:NE2	5:B:2023:HOH:O	2.29	0.65
1:A:90:ARG:HH11	1:A:90:ARG:HG2	1.62	0.65
1:A:214:VAL:O	1:A:218:GLU:HG3	1.97	0.65
2:W:3:DG:N2	3:X:22:DC:N3	2.42	0.64
1:B:195:LEU:O	1:B:200:GLN:NE2	2.24	0.64
1:B:177:ASN:HA	1:B:180:LEU:HD22	1.80	0.64
2:W:24:DA:C2	3:X:1:DT:N3	2.61	0.64
1:B:227:ASN:N	1:B:227:ASN:OD1	2.31	0.64
1:C:137:TYR:CE2	1:C:162:VAL:HG22	2.33	0.64
3:X:22:DC:H2'	3:X:23:DC:C6	2.32	0.64
1:A:212:LEU:HB3	1:A:216:GLN:HB2	1.81	0.63
1:A:67:HIS:ND1	1:A:70:LEU:HD12	2.13	0.63
1:C:85:ILE:HG12	1:C:86:ALA:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:4:DG:H2"	2:Z:5:DT:C5'	2.23	0.62
1:D:159:ARG:NH2	2:Z:6:DG:O6	2.29	0.62
1:B:46:TYR:CZ	1:B:51:VAL:HG13	2.35	0.62
1:C:42:MET:HB3	1:C:43:PRO:HD3	1.81	0.62
1:B:126:GLU:N	1:B:126:GLU:OE1	2.33	0.62
3:Y:4:DC:H2"	3:Y:5:DT:H5"	1.81	0.62
3:Y:12:DC:H2"	3:Y:13:DG:C8	2.35	0.62
3:X:8:DT:H1'	3:X:9:DT:H5'	1.82	0.61
1:A:213:SER:OG	1:A:216:GLN:HG3	2.01	0.61
1:D:222:ARG:HA	1:D:225:LYS:HD3	1.83	0.61
1:C:78:GLU:CB	1:C:87:GLY:H	2.13	0.61
1:D:144:TYR:HB2	1:D:146:MET:HG2	1.83	0.60
1:C:72:PRO:HB2	1:C:108:ASP:HB2	1.83	0.60
3:Y:1:DT:H2'	3:Y:2:DC:C6	2.35	0.60
1:A:88:GLU:OE1	1:A:92:ARG:NH1	2.33	0.60
1:D:99:MET:SD	1:D:100:PRO:HD2	2.40	0.60
1:A:103:LYS:HD2	5:A:2022:HOH:O	2.00	0.60
1:A:73:VAL:HG12	1:A:74:LEU:H	1.65	0.60
1:C:129:ASN:ND2	1:C:132:GLU:OE1	2.35	0.60
1:B:69:LEU:HD12	1:B:69:LEU:O	2.00	0.60
1:A:100:PRO:CD	1:A:101:THR:H	2.15	0.59
1:C:165:ILE:O	1:C:168:LEU:HB2	2.02	0.59
1:B:154:ILE:HG21	1:D:91:LEU:HD12	1.84	0.59
1:A:87:GLY:HA2	1:A:90:ARG:HD3	1.85	0.59
2:W:12:DC:H2"	2:W:13:DG:C8	2.37	0.59
1:B:62:GLN:HG2	1:B:96:LEU:HB2	1.85	0.58
2:W:22:DG:H1'	2:W:23:DG:C8	2.37	0.58
1:B:141:LEU:HD21	1:B:151:LEU:HD22	1.84	0.58
1:A:222:ARG:HH11	1:A:222:ARG:HB2	1.68	0.58
1:D:62:GLN:O	1:D:64:ILE:N	2.37	0.58
1:A:215:ARG:NH1	1:A:218:GLU:OE1	2.37	0.58
1:A:207:ILE:HA	1:A:212:LEU:HD12	1.85	0.58
1:A:100:PRO:HB2	1:A:103:LYS:NZ	2.19	0.57
1:C:54:GLU:N	1:C:54:GLU:OE1	2.36	0.57
1:A:86:ALA:H	1:C:83:HIS:CE1	2.21	0.57
1:C:203:ILE:O	1:C:207:ILE:HG13	2.03	0.57
1:C:76:VAL:HG12	1:C:77:SER:H	1.69	0.57
2:W:14:DT:H2"	2:W:15:DG:O4'	2.05	0.57
1:D:204:LEU:HA	1:D:207:ILE:HD12	1.85	0.57
1:B:66:GLU:OE2	1:B:69:LEU:HD22	2.04	0.57
1:B:66:GLU:HA	1:B:69:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:C	1:B:90:ARG:HE	2.08	0.57
1:C:125:ARG:HH21	1:C:127:ASP:CG	2.09	0.57
1:C:91:LEU:HG	1:C:92:ARG:N	2.18	0.57
1:D:67:HIS:HB3	5:D:2004:HOH:O	2.05	0.56
3:Y:24:DT:OP1	3:Y:24:DT:C4'	2.37	0.56
1:A:69:LEU:HB2	1:A:72:PRO:HA	1.86	0.56
1:A:144:TYR:CD1	1:C:89:ARG:HB2	2.41	0.56
3:Y:5:DT:H2"	3:Y:6:DG:H8	1.70	0.56
1:C:129:ASN:OD1	1:C:129:ASN:N	2.30	0.56
1:D:92:ARG:O	1:D:96:LEU:HG	2.05	0.56
1:B:74:LEU:HD13	1:B:90:ARG:NE	2.21	0.56
1:B:125:ARG:HA	1:B:125:ARG:HH11	1.71	0.56
2:W:2:DG:H8	5:W:2001:HOH:O	1.88	0.56
1:B:165:ILE:HD13	1:B:168:LEU:HD21	1.87	0.56
3:Y:3:DC:N4	2:Z:22:DG:H1	2.03	0.55
1:A:144:TYR:CG	1:C:89:ARG:HD2	2.40	0.55
1:A:69:LEU:N	1:A:69:LEU:HD13	2.22	0.55
1:A:141:LEU:HD21	1:A:151:LEU:HD22	1.88	0.55
1:A:84:LEU:HD11	1:A:87:GLY:HA3	1.88	0.55
1:C:123:ILE:HD12	1:C:140:LEU:HD12	1.88	0.55
1:A:89:ARG:HH21	1:B:89:ARG:NE	2.03	0.55
1:D:152:SER:HB3	1:D:157:LYS:O	2.07	0.55
1:A:172:SER:OG	1:A:174:LYS:NZ	2.40	0.55
1:D:131:LEU:HD12	1:D:180:LEU:HD21	1.88	0.55
1:C:191:VAL:HG11	1:C:218:GLU:HA	1.88	0.55
3:Y:22:DC:H2'	3:Y:23:DC:C6	2.41	0.54
1:B:46:TYR:CE1	1:B:51:VAL:HG13	2.42	0.54
1:A:90:ARG:CG	1:A:90:ARG:HH11	2.20	0.54
3:Y:5:DT:H2"	3:Y:6:DG:H5'	1.89	0.54
2:Z:4:DG:C2'	2:Z:5:DT:H5"	2.25	0.54
1:B:63:SER:N	1:B:99:MET:HE1	2.22	0.54
1:A:148:GLN:OE1	1:A:159:ARG:NH1	2.40	0.54
1:D:185:THR:OG1	1:D:188:HIS:ND1	2.32	0.54
1:A:67:HIS:HB2	1:A:70:LEU:CA	2.37	0.54
1:D:117:VAL:HA	1:D:120:ILE:HG22	1.90	0.54
3:Y:14:DT:H2'	3:Y:15:DG:C8	2.42	0.54
1:A:165:ILE:O	1:A:168:LEU:HB2	2.07	0.54
1:C:130:PRO:HG2	1:C:179:LEU:HD11	1.90	0.54
1:A:117:VAL:HG11	5:A:2034:HOH:O	2.07	0.54
1:C:98:LYS:HE3	1:C:101:THR:HA	1.88	0.54
1:B:50:LYS:HG2	1:D:110:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HH12	1:D:75:VAL:HG22	1.72	0.53
2:W:24:DA:N1	3:X:1:DT:C4	2.76	0.53
1:A:111:GLN:O	1:A:115:ARG:HG2	2.09	0.53
1:B:89:ARG:HB2	1:B:89:ARG:CZ	2.35	0.53
1:B:202:LEU:HD12	5:B:2039:HOH:O	2.07	0.53
1:C:181:GLU:HB3	1:C:183:LYS:HG2	1.90	0.53
1:B:74:LEU:HG	1:B:92:ARG:HH22	1.74	0.53
1:C:155:VAL:HG13	1:C:157:LYS:HG3	1.91	0.52
1:D:191:VAL:HG21	1:D:217:THR:HG22	1.90	0.52
1:B:84:LEU:H	1:B:84:LEU:HD23	1.75	0.52
2:W:22:DG:H2'	2:W:22:DG:OP2	2.08	0.52
1:A:195:LEU:O	1:A:200:GLN:NE2	2.42	0.52
1:B:92:ARG:HD2	1:B:93:ALA:N	2.25	0.52
1:C:85:ILE:HG12	1:C:86:ALA:N	2.24	0.52
1:A:59:GLU:HG2	1:A:93:ALA:HA	1.91	0.52
1:A:191:VAL:HG21	1:A:218:GLU:HA	1.91	0.52
1:A:74:LEU:HA	1:A:107:VAL:O	2.10	0.52
1:D:91:LEU:HD13	1:D:92:ARG:H	1.75	0.52
1:A:172:SER:HB3	1:A:175:VAL:HG23	1.91	0.52
1:D:65:LYS:HD3	1:D:67:HIS:HB2	1.91	0.51
3:X:17:DA:H1'	3:X:18:DA:H5'	1.92	0.51
1:A:188:HIS:O	1:A:191:VAL:HG12	2.11	0.51
3:Y:4:DC:C2'	3:Y:5:DT:H5"	2.41	0.51
1:B:47:GLN:HG3	1:B:48:PRO:HD2	1.92	0.51
1:C:149:GLU:O	1:C:153:LYS:HG2	2.10	0.51
1:B:123:ILE:HD12	1:D:92:ARG:NH2	2.25	0.51
1:B:116:GLU:O	1:B:120:ILE:HG23	2.10	0.51
1:C:57:LEU:HG	1:C:58:GLU:H	1.75	0.51
1:A:90:ARG:O	1:A:94:SER:HB2	2.10	0.51
2:Z:6:DG:C8	2:Z:6:DG:H5'	2.46	0.51
1:A:102:ILE:HG22	1:A:103:LYS:H	1.75	0.51
1:C:73:VAL:O	1:C:74:LEU:HD22	2.11	0.51
1:D:190:LYS:HE2	2:Z:9:DC:H41	1.74	0.51
2:W:3:DG:H2"	2:W:4:DG:H8	1.75	0.50
1:D:65:LYS:HG3	1:D:67:HIS:H	1.76	0.50
1:D:155:VAL:HG23	1:D:157:LYS:HB2	1.91	0.50
3:Y:15:DG:H2"	3:Y:16:DG:H5"	1.93	0.50
1:C:132:GLU:OE2	1:C:135:ARG:NH2	2.45	0.50
1:A:73:VAL:N	5:A:2004:HOH:O	2.41	0.50
1:B:74:LEU:N	1:B:90:ARG:HH21	2.02	0.50
1:D:144:TYR:N	1:D:144:TYR:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:SER:O	1:D:140:LEU:HB2	2.12	0.50
1:A:76:VAL:HG11	1:C:86:ALA:HB3	1.94	0.50
1:C:98:LYS:NZ	1:C:101:THR:HB	2.27	0.50
1:C:145:GLN:HA	1:C:145:GLN:OE1	2.12	0.50
1:A:167:ARG:NH2	2:W:7:DT:H2'	2.26	0.50
1:A:159:ARG:NH2	2:W:5:DT:H2'	2.23	0.50
1:A:62:GLN:HA	1:A:67:HIS:HE2	1.77	0.50
3:Y:24:DT:O4	2:Z:1:DA:N1	2.44	0.50
1:A:184:ILE:HD11	1:A:207:ILE:HG21	1.94	0.50
1:A:102:ILE:HG22	1:A:103:LYS:N	2.27	0.49
1:B:92:ARG:HH11	1:B:93:ALA:HB2	1.76	0.49
1:B:50:LYS:HE2	1:B:51:VAL:HG22	1.95	0.49
2:Z:21:DG:H2'	2:Z:22:DG:C8	2.47	0.49
1:B:104:ALA:HB1	5:B:2017:HOH:O	2.13	0.49
1:B:92:ARG:HD2	1:B:93:ALA:H	1.77	0.49
3:Y:3:DC:N3	2:Z:22:DG:N2	2.53	0.49
1:A:114:MET:HB3	1:A:115:ARG:HH21	1.77	0.49
1:A:129:ASN:ND2	5:A:2030:HOH:O	2.46	0.49
3:Y:14:DT:H2"	3:Y:15:DG:O4'	2.12	0.49
1:C:76:VAL:HG12	1:C:77:SER:N	2.27	0.49
1:B:199:LYS:HD3	1:B:224:PHE:HB3	1.94	0.49
1:A:99:MET:HB3	1:A:100:PRO:HD3	1.95	0.49
1:A:90:ARG:HD2	1:B:89:ARG:NH2	2.27	0.49
3:X:14:DT:H2"	3:X:15:DG:O5'	2.13	0.49
1:D:174:LYS:HD2	1:D:201:GLU:HG3	1.94	0.49
2:Z:8:DT:H2"	2:Z:9:DC:H5'	1.93	0.49
1:B:167:ARG:CZ	1:B:193:VAL:HG21	2.43	0.49
1:D:108:ASP:HB3	5:D:2011:HOH:O	2.13	0.49
1:B:49:ARG:NH1	5:B:2004:HOH:O	2.46	0.49
1:D:140:LEU:HD13	1:D:144:TYR:CE1	2.48	0.48
1:C:36:LEU:HD13	1:C:79:ASN:HB2	1.95	0.48
1:A:69:LEU:HD22	1:A:69:LEU:N	2.26	0.48
1:A:90:ARG:HG3	1:B:89:ARG:CZ	2.43	0.48
1:B:83:HIS:O	1:B:83:HIS:ND1	2.46	0.48
1:A:115:ARG:HA	1:A:115:ARG:NH1	2.29	0.48
1:A:96:LEU:H	1:A:96:LEU:HD22	1.77	0.48
1:A:89:ARG:NH2	1:B:92:ARG:HE	2.11	0.48
1:B:124:GLN:H	1:B:124:GLN:CD	2.17	0.48
5:W:2015:HOH:O	3:X:2:DC:N4	2.40	0.48
1:B:90:ARG:HB2	5:B:2012:HOH:O	2.13	0.48
1:C:111:GLN:O	1:C:115:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:NH2	5:C:2021:HOH:O	2.39	0.48
1:D:71:GLN:HG2	1:D:72:PRO:HD2	1.95	0.48
1:C:113:LYS:HZ3	1:C:114:MET:HB2	1.79	0.48
2:Z:6:DG:H8	2:Z:6:DG:H5'	1.79	0.47
1:B:74:LEU:HG	1:B:92:ARG:NH2	2.30	0.47
1:B:73:VAL:HG11	1:B:106:VAL:HB	1.97	0.47
1:A:74:LEU:HD12	1:B:72:PRO:HB3	1.95	0.47
1:B:141:LEU:O	1:B:145:GLN:HA	2.14	0.47
1:B:191:VAL:HG11	1:B:217:THR:HG22	1.97	0.47
1:D:52:PHE:CD1	1:D:52:PHE:N	2.80	0.47
1:A:99:MET:HE3	1:A:100:PRO:HD3	1.97	0.47
1:C:64:ILE:N	5:C:2008:HOH:O	2.47	0.47
1:D:119:LEU:O	1:D:123:ILE:HG22	2.14	0.47
1:A:146:MET:HG3	1:A:147:THR:N	2.30	0.47
1:B:56:SER:O	1:B:60:LEU:HB3	2.15	0.47
1:D:77:SER:OG	1:D:77:SER:O	2.28	0.47
1:B:203:ILE:O	1:B:207:ILE:HG13	2.14	0.47
1:D:68:GLY:HA2	1:D:104:ALA:C	2.35	0.47
1:D:127:ASP:OD1	1:D:129:ASN:N	2.48	0.47
1:A:73:VAL:HG22	1:A:90:ARG:HG2	1.96	0.47
1:A:215:ARG:HA	1:A:215:ARG:HD3	1.43	0.47
1:A:58:GLU:HG3	1:B:52:PHE:CD2	2.50	0.47
1:B:218:GLU:OE2	5:B:2037:HOH:O	2.21	0.47
2:Z:20:DA:H2'	5:Z:2012:HOH:O	2.15	0.47
2:Z:23:DG:H2"	5:Z:2013:HOH:O	2.15	0.46
1:A:162:VAL:O	1:A:166:MET:HG3	2.15	0.46
1:B:146:MET:HE2	1:B:150:GLU:HB2	1.97	0.46
1:D:101:THR:O	1:D:103:LYS:N	2.48	0.46
1:A:164:ASN:OD1	2:W:7:DT:H72	2.15	0.46
1:B:188:HIS:O	1:B:191:VAL:HG12	2.16	0.46
1:A:110:GLU:OE1	1:A:112:GLU:N	2.48	0.46
1:C:103:LYS:HB3	1:C:103:LYS:HE2	1.52	0.46
1:B:149:GLU:O	1:B:153:LYS:HG2	2.16	0.46
1:B:166:MET:O	1:B:169:LEU:HB2	2.15	0.46
1:A:117:VAL:O	1:A:121:GLU:HG2	2.15	0.46
1:D:195:LEU:O	1:D:200:GLN:NE2	2.42	0.46
1:D:187:GLY:O	1:D:191:VAL:HG13	2.15	0.46
1:A:71:GLN:OE1	1:B:74:LEU:HB2	2.15	0.46
1:D:101:THR:HG23	5:D:2010:HOH:O	2.15	0.46
1:C:110:GLU:HG3	1:C:113:LYS:HZ1	1.81	0.46
1:B:212:LEU:HD13	1:B:216:GLN:HB3	1.98	0.46

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:HE21	2:W:5:DT:H3'	1.78	0.46
3:X:10:DC:H1'	3:X:11:DA:N7	2.31	0.46
1:C:226:ILE:HG12	1:C:227:ASN:N	2.31	0.46
1:C:196:ASP:O	1:C:200:GLN:HG3	2.15	0.46
1:A:102:ILE:CD1	1:A:106:VAL:HG11	2.35	0.45
1:D:174:LYS:O	1:D:177:ASN:HB3	2.16	0.45
1:B:215:ARG:HA	1:B:215:ARG:HD3	1.75	0.45
1:A:73:VAL:HG11	1:A:84:LEU:HD11	1.97	0.45
1:B:62:GLN:O	1:B:66:GLU:HG2	2.17	0.45
1:B:167:ARG:NH1	1:B:193:VAL:HG21	2.31	0.45
1:B:216:GLN:O	1:B:219:ASP:N	2.50	0.45
1:D:132:GLU:OE1	1:D:135:ARG:NH2	2.48	0.45
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.77	0.45
2:Z:13:DG:H2"	2:Z:14:DT:OP2	2.16	0.45
1:A:69:LEU:HD12	1:A:90:ARG:HB3	1.99	0.45
2:W:2:DG:H2"	2:W:3:DG:C8	2.52	0.45
1:A:74:LEU:HD23	1:A:108:ASP:HA	1.98	0.45
1:A:69:LEU:CD2	1:A:69:LEU:H	2.21	0.45
1:A:91:LEU:O	1:A:94:SER:N	2.50	0.45
1:D:157:LYS:NZ	3:Y:15:DG:OP2	2.49	0.45
1:A:175:VAL:HG21	1:A:200:GLN:HG2	1.98	0.45
1:A:72:PRO:HB3	1:A:106:VAL:HB	1.99	0.45
1:C:42:MET:HE2	5:C:2036:HOH:O	2.17	0.45
1:D:103:LYS:O	1:D:106:VAL:N	2.50	0.45
3:X:13:DG:H2"	3:X:14:DT:O5'	2.16	0.45
1:D:149:GLU:HG2	1:D:149:GLU:H	1.46	0.45
1:B:129:ASN:HB3	1:B:132:GLU:HB2	1.98	0.45
1:B:95:LYS:O	1:B:98:LYS:HB3	2.16	0.45
1:C:165:ILE:HD12	1:C:165:ILE:HA	1.67	0.44
2:W:3:DG:H2"	2:W:4:DG:C8	2.52	0.44
1:A:75:VAL:HG23	1:A:108:ASP:HB2	2.00	0.44
3:Y:16:DG:H2'	3:Y:16:DG:H5'	1.71	0.44
1:C:71:GLN:OE1	1:C:74:LEU:HD21	2.18	0.44
1:C:132:GLU:HG3	1:C:135:ARG:NH2	2.32	0.44
1:D:79:ASN:HA	1:D:79:ASN:HD22	1.48	0.44
1:A:89:ARG:HG3	1:A:89:ARG:H	1.24	0.44
1:A:114:MET:HB3	1:A:115:ARG:NH2	2.33	0.44
1:D:225:LYS:HD2	5:D:2024:HOH:O	2.17	0.44
1:B:165:ILE:O	1:B:168:LEU:HG	2.17	0.44
1:B:74:LEU:H	1:B:90:ARG:NH2	2.04	0.44
3:Y:23:DC:H2"	3:Y:24:DT:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:CE	1:A:100:PRO:HD3	2.48	0.44
1:B:174:LYS:HD2	1:B:174:LYS:HA	1.84	0.44
1:B:58:GLU:HG2	1:B:62:GLN:HE22	1.81	0.44
3:Y:1:DT:H3	2:Z:24:DA:N6	2.16	0.44
1:D:203:ILE:HG22	1:D:207:ILE:HD11	1.99	0.44
1:B:92:ARG:H	1:B:92:ARG:HG3	1.53	0.43
1:A:144:TYR:CE2	1:A:146:MET:HB2	2.53	0.43
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.78	0.43
2:W:21:DG:N2	3:X:4:DC:N3	2.61	0.43
1:B:105:ILE:HG12	1:B:106:VAL:N	2.33	0.43
1:A:89:ARG:NH1	1:B:92:ARG:HG2	2.33	0.43
1:A:144:TYR:CZ	1:A:145:GLN:O	2.71	0.43
1:C:98:LYS:HE2	1:C:98:LYS:HB2	1.33	0.43
1:A:73:VAL:HG11	1:A:87:GLY:HA3	1.99	0.43
1:D:92:ARG:HA	1:D:92:ARG:HD3	1.76	0.43
1:D:134:ALA:HB1	1:D:169:LEU:HG	1.99	0.43
2:W:5:DT:H2"	2:W:6:DG:O5'	2.18	0.43
1:A:89:ARG:CZ	1:B:89:ARG:HH21	2.31	0.43
2:W:22:DG:H1	3:X:3:DC:H42	1.67	0.43
1:B:77:SER:HA	1:B:109:ILE:HD13	2.00	0.43
2:W:21:DG:H2"	2:W:22:DG:C8	2.54	0.43
1:B:68:GLY:O	1:B:70:LEU:HB2	2.19	0.43
1:A:199:LYS:HG2	1:A:199:LYS:H	1.56	0.43
3:Y:21:DC:H2'	3:Y:22:DC:C6	2.54	0.43
1:A:222:ARG:NH1	1:A:222:ARG:HB2	2.32	0.43
1:D:168:LEU:HA	1:D:168:LEU:HD12	1.78	0.43
1:D:61:ALA:C	1:D:63:SER:H	2.21	0.43
3:Y:7:DT:C2	3:Y:8:DT:C5	3.06	0.43
1:B:115:ARG:HD3	1:B:115:ARG:HA	1.65	0.43
1:A:144:TYR:CE1	1:C:89:ARG:HB2	2.54	0.43
1:B:85:ILE:CD1	1:B:90:ARG:HB3	2.47	0.43
1:B:115:ARG:NH1	1:D:75:VAL:HG22	2.34	0.43
1:C:70:LEU:HD13	1:C:71:GLN:HG3	2.00	0.43
3:X:20:DA:H2'	5:X:2005:HOH:O	2.18	0.43
1:C:141:LEU:HD21	1:C:148:GLN:HB3	2.01	0.43
2:Z:5:DT:H2"	2:Z:6:DG:H5'	2.00	0.42
1:A:148:GLN:HE22	2:W:5:DT:H3'	1.83	0.42
3:Y:15:DG:H2"	3:Y:16:DG:C8	2.53	0.42
1:C:70:LEU:HD22	1:C:71:GLN:N	2.31	0.42
1:C:129:ASN:HB2	5:C:2031:HOH:O	2.19	0.42
1:B:61:ALA:HB3	1:B:65:LYS:HZ1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:HG3	1:C:113:LYS:NZ	2.34	0.42
1:A:78:GLU:OE1	1:A:81:ARG:HB2	2.19	0.42
1:D:94:SER:C	1:D:95:LYS:HE3	2.39	0.42
3:Y:5:DT:H2"	3:Y:6:DG:C8	2.51	0.42
2:W:4:DG:H2'	2:W:5:DT:H71	2.02	0.42
2:Z:12:DC:H2'	2:Z:13:DG:C8	2.54	0.42
1:A:99:MET:HE3	1:A:99:MET:HB3	1.81	0.42
1:B:89:ARG:O	1:B:92:ARG:NE	2.52	0.42
3:Y:1:DT:H2'	3:Y:2:DC:C5	2.55	0.42
1:C:42:MET:CG	1:C:145:GLN:HB2	2.38	0.42
1:A:141:LEU:HD22	1:A:146:MET:HG2	2.00	0.42
1:D:74:LEU:HB3	1:D:83:HIS:CD2	2.55	0.42
1:A:71:GLN:HA	1:A:72:PRO:HD3	1.84	0.42
1:A:71:GLN:CD	1:B:74:LEU:HB2	2.40	0.42
1:D:146:MET:HB2	1:D:146:MET:HE3	1.91	0.42
1:C:64:ILE:HG12	5:C:2008:HOH:O	2.19	0.42
1:A:221:ALA:O	1:A:225:LYS:HD3	2.19	0.42
1:D:120:ILE:HD12	1:D:123:ILE:HG21	2.02	0.41
1:C:110:GLU:O	1:C:113:LYS:NZ	2.52	0.41
1:C:67:HIS:HA	5:C:2010:HOH:O	2.20	0.41
1:D:213:SER:OG	1:D:216:GLN:HG3	2.19	0.41
1:B:160:ALA:N	5:B:2030:HOH:O	2.50	0.41
1:B:137:TYR:O	1:B:141:LEU:HG	2.20	0.41
1:A:131:LEU:HB3	1:A:135:ARG:NH2	2.35	0.41
1:B:152:SER:HB2	1:B:157:LYS:O	2.20	0.41
1:C:95:LYS:HB2	1:C:95:LYS:HE2	1.90	0.41
3:X:21:DC:H2"	3:X:22:DC:O4'	2.20	0.41
1:A:100:PRO:CD	1:A:101:THR:N	2.82	0.41
1:D:52:PHE:HB2	1:D:54:GLU:OE2	2.21	0.41
1:D:151:LEU:O	1:D:155:VAL:HG13	2.20	0.41
1:B:62:GLN:C	1:B:99:MET:HE1	2.41	0.41
1:B:96:LEU:HA	5:B:2015:HOH:O	2.19	0.41
1:B:112:GLU:O	1:B:116:GLU:HB2	2.20	0.41
1:C:172:SER:HB3	1:C:200:GLN:OE1	2.20	0.41
2:Z:5:DT:H2"	2:Z:6:DG:C5'	2.51	0.41
1:A:69:LEU:HG	1:A:73:VAL:HG23	2.03	0.41
1:D:65:LYS:NZ	1:D:67:HIS:CG	2.89	0.41
1:D:176:GLN:O	1:D:180:LEU:HG	2.20	0.41
1:B:106:VAL:HG22	5:B:2018:HOH:O	2.21	0.41
1:A:71:GLN:HB2	1:B:75:VAL:HG12	2.02	0.41
1:B:66:GLU:HG3	1:B:99:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:12:DC:H2'	3:X:13:DG:C8	2.56	0.41
1:A:67:HIS:HD2	1:A:68:GLY:N	2.18	0.41
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.40	0.41
1:C:131:LEU:HB2	5:C:2031:HOH:O	2.21	0.41
1:C:177:ASN:O	1:C:181:GLU:HB2	2.21	0.41
1:D:190:LYS:CE	2:Z:9:DC:H41	2.34	0.41
1:B:106:VAL:O	1:B:107:VAL:HG12	2.21	0.41
1:A:110:GLU:HB3	1:A:113:LYS:HG3	2.03	0.41
1:D:213:SER:N	1:D:216:GLN:OE1	2.44	0.41
1:A:190:LYS:O	1:A:193:VAL:HG13	2.21	0.41
1:B:103:LYS:HB3	1:B:103:LYS:HE3	1.75	0.41
1:A:138:LYS:O	1:A:142:GLU:N	2.53	0.41
1:D:131:LEU:HD12	1:D:180:LEU:CD2	2.51	0.41
1:B:170:THR:O	1:B:170:THR:OG1	2.35	0.41
1:C:195:LEU:HD22	1:C:199:LYS:HD2	2.03	0.41
1:D:75:VAL:HG11	1:D:95:LYS:CE	2.47	0.40
1:A:141:LEU:C	1:A:144:TYR:O	2.59	0.40
1:B:108:ASP:N	1:B:108:ASP:OD1	2.52	0.40
1:D:52:PHE:N	1:D:52:PHE:HD1	2.19	0.40
1:B:138:LYS:HE2	1:B:169:LEU:HD12	2.03	0.40
1:C:52:PHE:CZ	1:C:70:LEU:HD21	2.57	0.40
1:A:184:ILE:HD11	1:A:207:ILE:CG2	2.51	0.40
3:Y:23:DC:C4	3:Y:24:DT:O4	2.75	0.40
1:C:80:GLY:HA2	1:C:85:ILE:HG22	2.04	0.40
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.85	0.40
1:C:46:TYR:HD1	1:C:46:TYR:H	1.70	0.40
1:A:89:ARG:NH2	1:B:89:ARG:HH21	2.18	0.40
1:A:90:ARG:HG3	1:B:89:ARG:NH1	2.37	0.40
1:B:57:LEU:HD12	1:B:58:GLU:H	1.86	0.40
1:B:50:LYS:HD3	1:B:51:VAL:N	2.37	0.40
1:B:115:ARG:CZ	1:D:76:VAL:HG23	2.52	0.40
1:A:140:LEU:HD13	1:A:151:LEU:HD13	2.04	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	170/240 (71%)	147 (86%)	18 (11%)	5 (3%)	6	29
1	B	181/240 (75%)	152 (84%)	24 (13%)	5 (3%)	6	30
1	C	191/240 (80%)	164 (86%)	19 (10%)	8 (4%)	3	19
1	D	174/240 (72%)	151 (87%)	18 (10%)	5 (3%)	6	29
All	All	716/960 (75%)	614 (86%)	79 (11%)	23 (3%)	5	26

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	LEU
1	C	81	ARG
1	D	63	SER
1	D	79	ASN
1	D	99	MET
1	D	102	ILE
1	A	101	THR
1	B	70	LEU
1	C	51	VAL
1	A	99	MET
1	B	142	GLU
1	C	76	VAL
1	A	68	GLY
1	B	220	LEU
1	C	50	LYS
1	C	97	ALA
1	B	221	ALA
1	C	80	GLY
1	C	85	ILE
1	C	100	PRO
1	A	216	GLN
1	A	80	GLY
1	D	80	GLY

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	153/212 (72%)	112 (73%)	41 (27%)	0	1	
1	B	164/212 (77%)	116 (71%)	48 (29%)	0	1	
1	C	172/212 (81%)	119 (69%)	53 (31%)	0	1	
1	D	157/212 (74%)	106 (68%)	51 (32%)	0	0	
All	All	646/848 (76%)	453 (70%)	193 (30%)	0	1	

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	64	ILE
1	A	67	HIS
1	A	69	LEU
1	A	74	LEU
1	A	76	VAL
1	A	88	GLU
1	A	89	ARG
1	A	90	ARG
1	A	91	LEU
1	A	94	SER
1	A	95	LYS
1	A	98	LYS
1	A	102	ILE
1	A	103	LYS
1	A	105	ILE
1	A	107	VAL
1	A	108	ASP
1	A	114	MET
1	A	119	LEU
1	A	124	GLN
1	A	125	ARG
1	A	128	LEU
1	A	132	GLU
1	A	141	LEU
1	A	144	TYR
1	A	145	GLN
1	A	147	THR

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Mol	Chain	Res	Type
1	A	159	ARG
1	A	176	GLN
1	A	180	LEU
1	A	182	GLU
1	A	183	LYS
1	A	191	VAL
1	A	193	VAL
1	A	196	ASP
1	A	199	LYS
1	A	200	GLN
1	A	202	LEU
1	A	215	ARG
1	A	222	ARG
1	B	46	TYR
1	B	50	LYS
1	B	54	GLU
1	B	57	LEU
1	B	58	GLU
1	B	62	GLN
1	B	64	ILE
1	B	67	HIS
1	B	70	LEU
1	B	71	GLN
1	B	73	VAL
1	B	74	LEU
1	B	76	VAL
1	B	81	ARG
1	B	89	ARG
1	B	90	ARG
1	B	91	LEU
1	B	94	SER
1	B	96	LEU
1	B	98	LYS
1	B	99	MET
1	B	101	THR
1	B	103	LYS
1	B	105	ILE
1	B	106	VAL
1	B	109	ILE
1	B	113	LYS
1	B	114	MET
1	B	115	ARG

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Mol	Chain	Res	Type
1	B	116	GLU
1	B	120	ILE
1	B	122	ASN
1	B	124	GLN
1	B	125	ARG
1	B	128	LEU
1	B	150	GLU
1	B	165	ILE
1	B	168	LEU
1	B	180	LEU
1	B	183	LYS
1	B	196	ASP
1	B	208	ILE
1	B	211	LYS
1	B	215	ARG
1	B	220	LEU
1	B	225	LYS
1	B	226	ILE
1	B	227	ASN
1	C	39	ASP
1	C	46	TYR
1	C	58	GLU
1	C	59	GLU
1	C	60	LEU
1	C	62	GLN
1	C	64	ILE
1	C	66	GLU
1	C	67	HIS
1	C	69	LEU
1	C	70	LEU
1	C	71	GLN
1	C	73	VAL
1	C	77	SER
1	C	78	GLU
1	C	81	ARG
1	C	82	TYR
1	C	85	ILE
1	C	88	GLU
1	C	90	ARG
1	C	91	LEU
1	C	92	ARG
1	C	95	LYS

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Mol	Chain	Res	Type
1	C	98	LYS
1	C	102	ILE
1	C	103	LYS
1	C	105	ILE
1	C	110	GLU
1	C	113	LYS
1	C	115	ARG
1	C	123	ILE
1	C	126	GLU
1	C	129	ASN
1	C	132	GLU
1	C	139	GLU
1	C	141	LEU
1	C	143	SER
1	C	145	GLN
1	C	147	THR
1	C	149	GLU
1	C	151	LEU
1	C	156	LYS
1	C	157	LYS
1	C	159	ARG
1	C	165	ILE
1	C	172	SER
1	C	173	SER
1	C	179	LEU
1	C	201	GLU
1	C	206	SER
1	C	215	ARG
1	C	225	LYS
1	C	226	ILE
1	D	52	PHE
1	D	54	GLU
1	D	55	ASP
1	D	59	GLU
1	D	62	GLN
1	D	63	SER
1	D	64	ILE
1	D	65	LYS
1	D	66	GLU
1	D	67	HIS
1	D	70	LEU
1	D	73	VAL

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Mol	Chain	Res	Type
1	D	74	LEU
1	D	75	VAL
1	D	76	VAL
1	D	77	SER
1	D	79	ASN
1	D	81	ARG
1	D	85	ILE
1	D	90	ARG
1	D	91	LEU
1	D	92	ARG
1	D	95	LYS
1	D	96	LEU
1	D	99	MET
1	D	100	PRO
1	D	103	LYS
1	D	105	ILE
1	D	108	ASP
1	D	113	LYS
1	D	115	ARG
1	D	123	ILE
1	D	124	GLN
1	D	126	GLU
1	D	127	ASP
1	D	132	GLU
1	D	140	LEU
1	D	143	SER
1	D	144	TYR
1	D	146	MET
1	D	147	THR
1	D	148	GLN
1	D	149	GLU
1	D	150	GLU
1	D	151	LEU
1	D	186	SER
1	D	196	ASP
1	D	202	LEU
1	D	215	ARG
1	D	216	GLN
1	D	226	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	D	79	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	SO4	A	1227	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	A	1228	-	4,4,4	0.23	0	6,6,6	0.14	0
4	SO4	B	1228	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	C	1228	-	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	D	1227	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	W	1025	-	4,4,4	0.22	0	6,6,6	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1227	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1228	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1228	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1228	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1227	-	-	0/0/0/0	0/0/0/0
4	SO4	W	1025	-	-	0/0/0/0	0/0/0/0

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	172/240 (71%)	0.27	7 (4%)	41	19	23, 62, 107, 140	0
1	B	183/240 (76%)	0.51	20 (10%)	7	2	28, 71, 112, 142	0
1	C	193/240 (80%)	0.70	25 (12%)	5	2	24, 67, 126, 146	0
1	D	176/240 (73%)	0.78	23 (13%)	5	2	24, 70, 126, 137	0
2	W	24/24 (100%)	-0.12	0	100	100	27, 45, 84, 97	0
2	Z	24/24 (100%)	-0.30	0	100	100	26, 48, 109, 126	0
3	X	24/24 (100%)	-0.24	0	100	100	30, 51, 97, 102	0
3	Y	24/24 (100%)	-0.23	0	100	100	29, 59, 99, 106	0
All	All	820/1056 (77%)	0.48	75 (9%)	11	4	23, 65, 122, 146	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	LEU	12.1
1	D	89	ARG	9.1
1	C	97	ALA	8.6
1	C	47	GLN	8.5
1	D	87	GLY	7.3
1	D	72	PRO	7.0
1	C	100	PRO	6.9
1	D	105	ILE	6.8
1	D	73	VAL	6.7
1	C	44	ASN	6.6
1	C	85	ILE	6.4
1	C	48	PRO	6.3
1	B	59	GLU	6.3
1	C	96	LEU	6.1
1	D	85	ILE	6.0
1	D	93	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	83	HIS	4.8
1	B	60	LEU	4.8
1	A	67	HIS	4.7
1	C	98	LYS	4.6
1	C	50	LYS	4.4
1	C	107	VAL	4.4
1	B	96	LEU	4.3
1	D	88	GLU	4.2
1	C	81	ARG	4.2
1	C	46	TYR	4.1
1	D	86	ALA	3.9
1	D	123	ILE	3.8
1	C	106	VAL	3.5
1	D	52	PHE	3.5
1	D	67	HIS	3.4
1	C	101	THR	3.4
1	C	83	HIS	3.4
1	D	74	LEU	3.4
1	D	94	SER	3.3
1	C	103	LYS	3.3
1	B	69	LEU	3.3
1	B	70	LEU	3.3
1	A	143	SER	3.3
1	C	45	PRO	3.2
1	D	144	TYR	3.2
1	C	111	GLN	3.2
1	D	68	GLY	3.2
1	D	75	VAL	3.2
1	A	116	GLU	3.1
1	B	94	SER	3.1
1	C	53	SER	2.9
1	B	63	SER	2.9
1	C	58	GLU	2.9
1	B	108	ASP	2.8
1	A	109	ILE	2.7
1	B	52	PHE	2.7
1	D	57	LEU	2.7
1	A	79	ASN	2.6
1	B	61	ALA	2.6
1	B	64	ILE	2.6
1	B	53	SER	2.5
1	C	38	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	73	VAL	2.5
1	B	78	GLU	2.5
1	B	86	ALA	2.5
1	D	128	LEU	2.4
1	C	43	PRO	2.4
1	D	108	ASP	2.4
1	D	70	LEU	2.4
1	B	88	GLU	2.4
1	A	62	GLN	2.3
1	C	40	GLU	2.3
1	B	144	TYR	2.2
1	B	89	ARG	2.2
1	C	93	ALA	2.2
1	B	49	ARG	2.2
1	C	70	LEU	2.2
1	B	68	GLY	2.1
1	A	101	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
4	SO4	B	1228	5/5	0.68	0.47	4.17	131,132,134,141	0
4	SO4	W	1025	5/5	0.80	0.19	0.34	124,124,129,132	0
4	SO4	A	1227	5/5	0.80	0.21	-0.85	121,123,124,129	0
4	SO4	C	1228	5/5	0.76	0.17	-1.34	149,149,152,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	SO4	D	1227	5/5	0.84	0.18	-	85,96,98,103	0
4	SO4	A	1228	5/5	0.69	0.22	-	106,115,123,127	0

6.5 Other polymers (i)

There are no such residues in this entry.