Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:57 PM GMT

PDB ID	:	1MUH
Title	:	CRYSTAL STRUCTURE OF TN5 TRANSPOSASE COMPLEXED WITH TRANSPOSON END DNA
Authors	:	Thoden, J.B.; Holden, H.M.; Davies, D.R.; Goryshin, I.Y.; Reznikoff, W.S.; Rayment, I.
Deposited on	:	2002-09-23
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

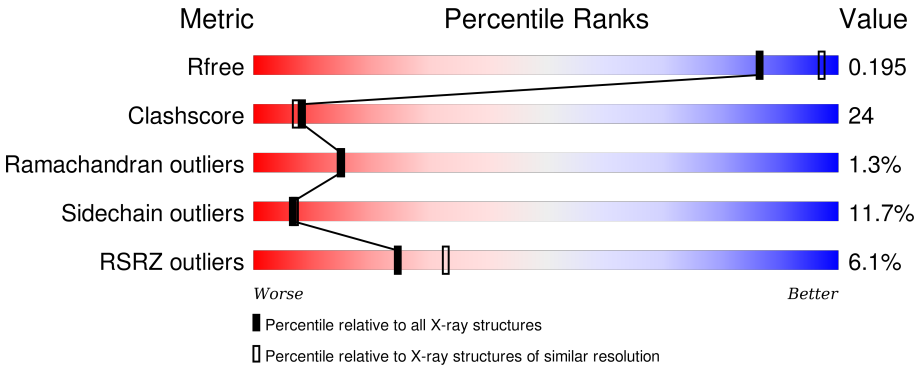
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	B	20	10%, 5%, 45%, 45%, 5%
2	C	20	5%, 10%, 35%, 50%, 5%
3	A	481	6%, 45%, 39%, 10%, • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4691 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 DNA TRANSFERRED STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	20	Total	C	N	O	P	0	0	0
			413	198	78	118	19			

- Molecule 2 is a DNA chain called DNA NON-TRANSFERRED STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			401	194	70	118	19			

- Molecule 3 is a protein called Tn5 transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	455	Total	C	N	O	S	0	1	0
			3569	2250	653	654	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LYS	GLU	ENGINEERED	UNP Q46731
A	56	ALA	MET	ENGINEERED	UNP Q46731
A	372	PRO	LEU	ENGINEERED	UNP Q46731
A	477	GLY	-	CLONING ARTIFACT	UNP Q46731

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

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

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

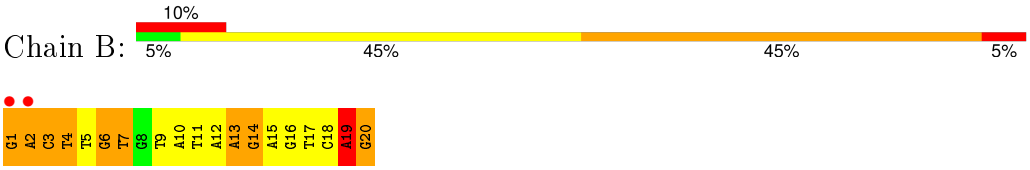
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	27	Total O 27 27	0	0
6	C	22	Total O 22 22	0	0
6	A	257	Total O 257 257	0	0

3 Residue-property plots (i)

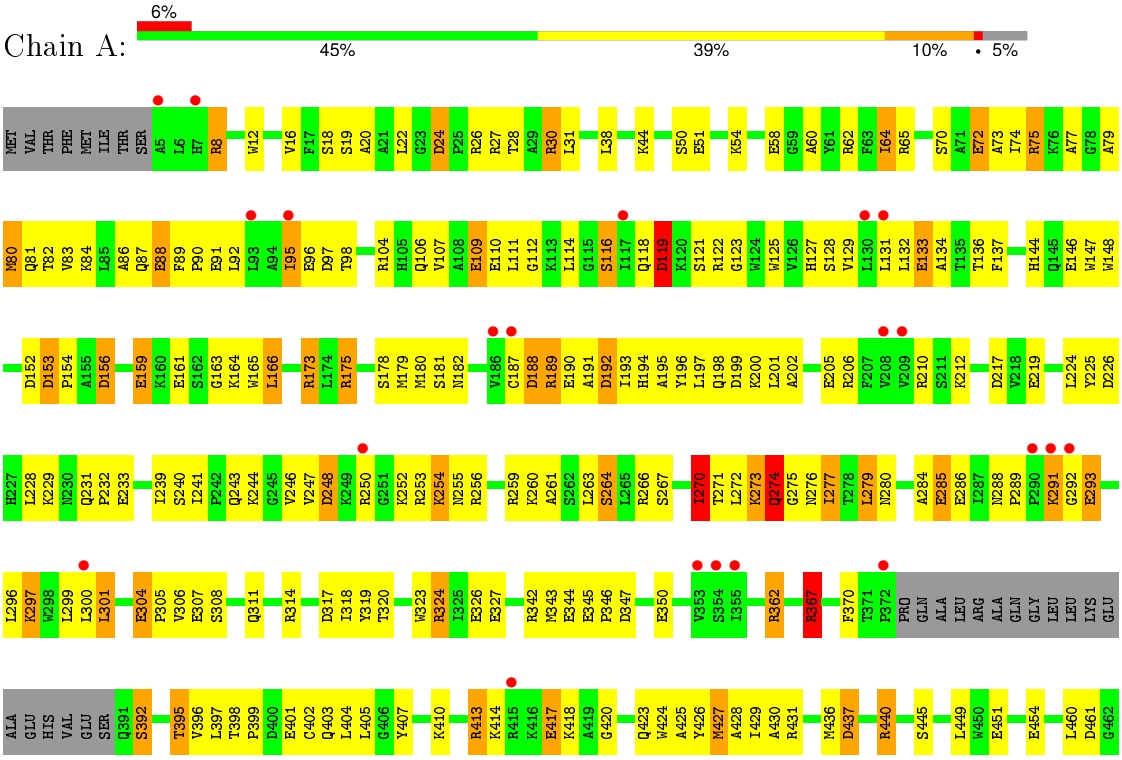
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

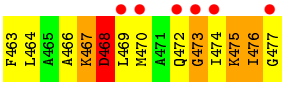
- Molecule 1: DNA TRANSFERRED STRAND



- Molecule 2: DNA NON-TRANSFERRED STRAND

- Molecule 3: Tn5 transposase




F463
L464
A465
A466
K467
D468
L469
M470
A471
Q472
G473
T474
K475
T476
G477

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	113.70Å 113.70Å 228.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 28.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.30) 99.8 (28.84-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 2.31Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.204 , 0.267 0.199 , 0.195	Depositor DCC
R_{free} test set	4023 reflections (11.37%)	DCC
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 115.5	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 39412 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4691	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

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

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	B	1.55	3/464 (0.6%)	2.58	38/716 (5.3%)
2	C	1.40	2/448 (0.4%)	2.64	49/688 (7.1%)
3	A	1.08	25/3642 (0.7%)	1.63	66/4914 (1.3%)
All	All	1.17	30/4554 (0.7%)	1.89	153/6318 (2.4%)

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	B	0	1
2	C	0	1
All	All	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	DT	C3'-O3'	-8.43	1.32	1.44
3	A	326	GLU	CD-OE2	8.10	1.34	1.25
3	A	219	GLU	CD-OE2	8.01	1.34	1.25
3	A	72	GLU	CD-OE2	7.97	1.34	1.25
3	A	285	GLU	CD-OE2	7.37	1.33	1.25
3	A	159	GLU	CD-OE2	7.05	1.33	1.25
3	A	454	GLU	CD-OE2	6.86	1.33	1.25
3	A	417	GLU	CD-OE2	6.68	1.33	1.25
3	A	88	GLU	CD-OE2	6.62	1.32	1.25
3	A	233	GLU	CD-OE2	6.58	1.32	1.25
3	A	161	GLU	CD-OE2	6.42	1.32	1.25
1	B	19	DA	P-O5'	6.27	1.66	1.59
3	A	345	GLU	CD-OE2	6.25	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	DT	C3'-O3'	-6.15	1.35	1.44
3	A	58	GLU	CD-OE2	6.06	1.32	1.25
3	A	96	GLU	CD-OE2	5.98	1.32	1.25
3	A	293	GLU	CD-OE2	5.94	1.32	1.25
3	A	110	GLU	CD-OE2	5.93	1.32	1.25
3	A	109	GLU	CD-OE2	5.93	1.32	1.25
2	C	5	DC	C3'-O3'	-5.89	1.36	1.44
3	A	307	GLU	CD-OE2	5.86	1.32	1.25
3	A	451	GLU	CD-OE2	5.84	1.32	1.25
3	A	304	GLU	CD-OE2	5.82	1.32	1.25
3	A	190	GLU	CD-OE2	5.79	1.32	1.25
3	A	133	GLU	CD-OE2	5.75	1.31	1.25
3	A	327	GLU	CD-OE2	5.69	1.31	1.25
3	A	146	GLU	CD-OE2	5.62	1.31	1.25
3	A	286	GLU	CD-OE2	5.59	1.31	1.25
2	C	14	DA	C3'-O3'	-5.31	1.37	1.44
3	A	344	GLU	CD-OE2	5.27	1.31	1.25

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	DA	C4-N9-C1'	-15.76	97.94	126.30
1	B	1	DG	C4-N9-C1'	-15.43	106.44	126.50
1	B	1	DG	C8-N9-C1'	14.55	145.92	127.00
1	B	19	DA	C8-N9-C1'	11.91	149.14	127.70
2	C	8	DT	O4'-C1'-N1	-11.83	99.72	108.00
1	B	6	DG	O4'-C1'-N9	-11.62	99.87	108.00
2	C	18	DG	C4-N9-C1'	-10.57	112.76	126.50
3	A	62	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	B	5	DT	P-O3'-C3'	9.95	131.64	119.70
2	C	2	DT	C6-N1-C1'	-9.75	105.77	120.40
3	A	342	ARG	NE-CZ-NH1	9.49	125.05	120.30
2	C	4	DA	C8-N9-C1'	9.47	144.75	127.70
3	A	24	ASP	CB-CG-OD1	9.31	126.68	118.30
3	A	342	ARG	NE-CZ-NH2	-9.28	115.66	120.30
3	A	24	ASP	CB-CG-OD2	-9.22	110.00	118.30
2	C	18	DG	C8-N9-C1'	9.12	138.85	127.00
2	C	15	DC	O4'-C1'-N1	8.96	114.27	108.00
1	B	20	DG	O4'-C4'-C3'	-8.91	100.66	106.00
2	C	11	DT	O4'-C1'-N1	8.91	114.23	108.00
2	C	1	DC	C2-N1-C1'	8.89	128.58	118.80
2	C	4	DA	C4-N9-C1'	-8.74	110.57	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	217	ASP	CB-CG-OD1	8.59	126.03	118.30
3	A	173	ARG	NE-CZ-NH2	-8.54	116.03	120.30
3	A	217	ASP	CB-CG-OD2	-8.45	110.69	118.30
2	C	15	DC	P-O5'-C5'	-8.34	107.55	120.90
3	A	65	ARG	NE-CZ-NH1	8.33	124.46	120.30
2	C	18	DG	P-O5'-C5'	-8.27	107.67	120.90
3	A	461	ASP	CB-CG-OD1	8.24	125.72	118.30
2	C	1	DC	C6-N1-C1'	-8.20	110.96	120.80
1	B	19	DA	O4'-C1'-N9	7.99	113.59	108.00
2	C	2	DT	C2-N1-C1'	7.96	130.94	118.20
1	B	2	DA	C4-N9-C1'	-7.93	112.02	126.30
3	A	362	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	4	DT	C6-N1-C1'	-7.81	108.68	120.40
3	A	362	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	4	DT	C2-N1-C1'	7.78	130.66	118.20
2	C	11	DT	P-O3'-C3'	7.67	128.91	119.70
2	C	2	DT	O4'-C1'-N1	-7.59	102.69	108.00
3	A	226	ASP	CB-CG-OD2	-7.53	111.52	118.30
3	A	75	ARG	NE-CZ-NH1	7.49	124.04	120.30
3	A	461	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	B	4	DT	O4'-C1'-N1	7.45	113.22	108.00
2	C	2	DT	C5'-C4'-C3'	7.42	127.45	114.10
2	C	4	DA	O4'-C1'-N9	7.39	113.17	108.00
3	A	97	ASP	CB-CG-OD1	7.36	124.92	118.30
2	C	10	DA	C8-N9-C4	7.32	108.73	105.80
3	A	75	ARG	NE-CZ-NH2	-7.29	116.65	120.30
2	C	20	DC	C6-N1-C2	7.21	123.18	120.30
1	B	5	DT	C2-N1-C1'	-7.19	106.69	118.20
1	B	14	DG	P-O5'-C5'	-7.18	109.40	120.90
3	A	199	ASP	CB-CG-OD2	-7.18	111.84	118.30
3	A	97	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	9	DT	C6-N1-C1'	-7.00	109.91	120.40
3	A	437	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	2	DA	C8-N9-C1'	6.96	140.23	127.70
1	B	11	DT	P-O3'-C3'	-6.88	111.45	119.70
3	A	153	ASP	CB-CG-OD2	-6.85	112.13	118.30
3	A	89	PHE	CB-CG-CD2	-6.84	116.02	120.80
2	C	18	DG	P-O3'-C3'	-6.79	111.55	119.70
3	A	317	ASP	CB-CG-OD2	-6.76	112.21	118.30
3	A	248	ASP	CB-CG-OD1	6.73	124.36	118.30
2	C	13	DC	P-O5'-C5'	-6.58	110.36	120.90
3	A	271	THR	CA-CB-CG2	-6.55	103.24	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	DT	C4'-C3'-C2'	-6.53	97.22	103.10
3	A	192	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	2	DA	O4'-C1'-C2'	6.52	111.12	105.90
3	A	317	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	4	DT	C5'-C4'-C3'	-6.47	102.45	114.10
1	B	4	DT	C4'-C3'-C2'	-6.45	97.30	103.10
3	A	128	SER	CB-CA-C	-6.44	97.86	110.10
2	C	7	DC	C6-N1-C2	6.43	122.87	120.30
3	A	119	ASP	CB-CG-OD2	-6.43	112.51	118.30
2	C	16	DA	P-O3'-C3'	6.40	127.38	119.70
1	B	18	DC	N3-C4-C5	6.38	124.45	121.90
2	C	5	DC	P-O5'-C5'	-6.37	110.71	120.90
2	C	5	DC	C5-C6-N1	-6.36	117.82	121.00
3	A	153	ASP	CB-CG-OD1	6.36	124.02	118.30
3	A	440	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	15	DA	O4'-C1'-N9	-6.30	103.59	108.00
2	C	9	DT	C6-N1-C2	6.28	124.44	121.30
2	C	7	DC	O4'-C1'-N1	-6.25	103.63	108.00
3	A	189	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	C	15	DC	C4'-C3'-C2'	-6.15	97.56	103.10
2	C	11	DT	C4-C5-C7	6.15	122.69	119.00
3	A	62	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	C	17	DA	O4'-C1'-C2'	-6.08	101.03	105.90
1	B	3	DC	C2-N1-C1'	-6.04	112.16	118.80
3	A	210	ARG	NE-CZ-NH2	-6.03	117.28	120.30
3	A	250	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	16	DG	O4'-C1'-N9	-6.01	103.80	108.00
3	A	256	ARG	CA-CB-CG	-6.00	100.21	113.40
3	A	119	ASP	CB-CG-OD1	5.93	123.64	118.30
2	C	10	DA	P-O5'-C5'	-5.93	111.41	120.90
3	A	199	ASP	CB-CG-OD1	5.92	123.63	118.30
3	A	192	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	C	5	DC	O4'-C4'-C3'	-5.90	102.14	104.50
1	B	13	DA	P-O3'-C3'	-5.90	112.62	119.70
1	B	18	DC	O4'-C1'-C2'	-5.88	101.20	105.90
2	C	8	DT	C5-C6-N1	-5.85	120.19	123.70
3	A	266	ARG	NE-CZ-NH1	5.83	123.22	120.30
2	C	15	DC	C6-N1-C2	5.82	122.63	120.30
3	A	8	ARG	CD-NE-CZ	5.78	131.69	123.60
2	C	20	DC	O4'-C4'-C3'	-5.75	102.20	104.50
3	A	250	ARG	NE-CZ-NH1	5.73	123.16	120.30
3	A	152	ASP	CB-CG-OD2	-5.72	113.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	DG	C8-N9-C4	5.68	108.67	106.40
3	A	248	ASP	CB-CG-OD2	-5.68	113.19	118.30
3	A	427	MET	CA-CB-CG	-5.66	103.68	113.30
2	C	10	DA	N9-C4-C5	-5.62	103.55	105.80
3	A	274	GLN	C-N-CA	-5.60	110.54	122.30
2	C	7	DC	C2-N1-C1'	-5.55	112.69	118.80
2	C	8	DT	C6-N1-C1'	-5.53	112.11	120.40
1	B	5	DT	C6-N1-C1'	5.53	128.69	120.40
3	A	253	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	A	347	ASP	CB-CG-OD2	-5.49	113.36	118.30
3	A	156	ASP	CB-CG-OD2	-5.47	113.38	118.30
3	A	324	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	C	20	DC	C3'-C2'-C1'	-5.45	95.96	102.50
3	A	147	TRP	CB-CA-C	-5.45	99.50	110.40
3	A	64	ILE	C-N-CA	-5.43	108.12	121.70
1	B	20	DG	O4'-C1'-N9	-5.43	104.20	108.00
3	A	347	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	4	DT	C6-C5-C7	-5.39	119.67	122.90
3	A	210	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	C	17	DA	C1'-O4'-C4'	-5.38	104.72	110.10
3	A	175	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	A	468	ASP	CB-CG-OD2	-5.36	113.47	118.30
2	C	9	DT	P-O3'-C3'	5.36	126.13	119.70
2	C	11	DT	C6-N1-C2	5.35	123.98	121.30
3	A	8	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	20	DG	C8-N9-C1'	-5.34	120.06	127.00
3	A	256	ARG	N-CA-CB	5.31	120.16	110.60
3	A	189	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	C	14	DA	C3'-C2'-C1'	-5.28	96.16	102.50
2	C	9	DT	C6-C5-C7	-5.26	119.75	122.90
3	A	324	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	9	DT	C2-N1-C1'	5.20	126.52	118.20
1	B	17	DT	C4'-C3'-C2'	5.20	107.78	103.10
1	B	18	DC	N3-C4-N4	-5.16	114.39	118.00
1	B	18	DC	C6-N1-C2	5.14	122.36	120.30
1	B	5	DT	C6-N1-C2	5.14	123.87	121.30
1	B	13	DA	C4-N9-C1'	-5.13	117.06	126.30
1	B	10	DA	C8-N9-C4	5.13	107.85	105.80
3	A	407	TYR	CB-CG-CD1	5.12	124.07	121.00
3	A	173	ARG	CB-CA-C	-5.11	100.19	110.40
2	C	5	DC	C1'-O4'-C4'	-5.10	105.00	110.10
3	A	270	ILE	CB-CA-C	-5.08	101.43	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	DC	O4'-C1'-C2'	5.07	109.96	105.90
2	C	15	DC	C5'-C4'-O4'	-5.07	99.67	109.30
2	C	7	DC	P-O5'-C5'	-5.06	112.81	120.90
3	A	413	ARG	NE-CZ-NH2	-5.01	117.79	120.30
3	A	367	ARG	CD-NE-CZ	-5.01	116.58	123.60
3	A	468	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	DA	Sidechain
2	C	11	DT	Sidechain

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	B	413	0	227	12	0
2	C	401	0	228	22	0
3	A	3569	0	3601	175	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	257	0	0	7	0
6	B	27	0	0	0	0
6	C	22	0	0	3	0
All	All	4691	0	4056	203	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 24.

All (203) 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:A:189:ARG:HB3	3:A:212:LYS:HB2	1.22	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:HIS:CD2	3:A:274:GLN:HG3	2.02	0.94
1:B:4:DT:H5"	1:B:4:DT:H6	1.31	0.94
3:A:194:HIS:CE1	3:A:274:GLN:HB2	2.08	0.88
3:A:472:GLN:HG3	3:A:474:ILE:HD11	1.55	0.88
3:A:189:ARG:CB	3:A:212:LYS:HB2	2.04	0.88
3:A:472:GLN:HG3	3:A:474:ILE:CD1	2.07	0.82
1:B:4:DT:C6	1:B:4:DT:H5"	2.16	0.80
2:C:14:DA:H1'	2:C:15:DC:H5"	1.61	0.80
3:A:189:ARG:HB3	3:A:212:LYS:CB	2.10	0.79
3:A:308:SER:OG	3:A:311:GLN:HG3	1.84	0.77
3:A:107:VAL:HG23	3:A:346:PRO:HD3	1.65	0.77
3:A:370:PHE:HE2	3:A:396:VAL:HG11	1.51	0.76
3:A:367:ARG:HB2	3:A:449:LEU:HD12	1.67	0.75
2:C:14:DA:H1'	2:C:15:DC:C5'	2.20	0.71
3:A:22:LEU:HD12	3:A:28:THR:HA	1.73	0.70
2:C:5:DC:OP1	3:A:367:ARG:NH2	2.25	0.70
2:C:17:DA:H2'	6:C:195:HOH:O	1.91	0.70
3:A:106:GLN:O	3:A:109:GLU:HG3	1.90	0.70
3:A:370:PHE:CE2	3:A:396:VAL:HG11	2.26	0.69
3:A:426:TYR:HD2	3:A:427:MET:HG2	1.56	0.69
3:A:468:ASP:O	3:A:472:GLN:HG2	1.93	0.68
3:A:414:LYS:O	3:A:417:GLU:HG2	1.93	0.68
3:A:8:ARG:HH12	3:A:401:GLU:CD	1.97	0.67
3:A:106:GLN:HG3	6:A:678:HOH:O	1.94	0.67
3:A:260:LYS:NZ	3:A:260:LYS:HB3	2.10	0.66
3:A:75:ARG:NH2	3:A:350:GLU:OE2	2.28	0.66
3:A:398:THR:OG1	3:A:401:GLU:HG2	1.96	0.66
3:A:473:GLY:C	3:A:474:ILE:HG13	2.17	0.65
3:A:244:LYS:HE2	3:A:246:VAL:CG1	2.27	0.65
3:A:20:ALA:HB3	3:A:28:THR:HG23	1.78	0.65
3:A:464:LEU:N	3:A:464:LEU:HD23	2.12	0.63
3:A:188:ASP:HB2	6:A:579:HOH:O	2.00	0.62
3:A:22:LEU:HD12	3:A:28:THR:CA	2.30	0.61
3:A:231:GLN:HB3	3:A:232:PRO:HD2	1.83	0.60
3:A:20:ALA:HA	3:A:77:ALA:HB2	1.83	0.60
3:A:473:GLY:O	3:A:474:ILE:HG13	2.01	0.59
3:A:194:HIS:NE2	3:A:274:GLN:HG3	2.18	0.59
3:A:31:LEU:O	3:A:31:LEU:HD12	2.04	0.58
3:A:392:SER:O	3:A:395:THR:OG1	2.18	0.58
3:A:70:SER:O	3:A:74:ILE:HG13	2.04	0.58
3:A:476:ILE:HG12	3:A:477:GLY:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:84:LYS:O	3:A:87:GLN:HB2	2.04	0.58
3:A:398:THR:O	3:A:402:CYS:HB2	2.04	0.58
3:A:91:GLU:HB3	3:A:134:ALA:HB3	1.84	0.57
3:A:466:ALA:O	3:A:467:LYS:C	2.41	0.57
2:C:14:DA:C1'	2:C:15:DC:H5"	2.31	0.57
3:A:107:VAL:CG2	3:A:346:PRO:HD3	2.34	0.57
3:A:426:TYR:CE1	3:A:449:LEU:HD11	2.40	0.57
3:A:193:ILE:HG22	3:A:196:TYR:H	1.70	0.56
3:A:314:ARG:HA	6:A:675:HOH:O	2.03	0.56
3:A:194:HIS:NE2	3:A:274:GLN:HB2	2.21	0.55
3:A:8:ARG:NH2	3:A:401:GLU:OE2	2.35	0.55
3:A:425:ALA:O	3:A:429:ILE:HG13	2.07	0.54
3:A:173:ARG:HA	3:A:180:MET:CG	2.37	0.54
3:A:112:GLY:O	3:A:122:ARG:HB3	2.08	0.54
3:A:398:THR:HB	3:A:399:PRO:HD2	1.89	0.54
3:A:244:LYS:HE2	3:A:246:VAL:HG12	1.88	0.54
2:C:2:DT:H3'	2:C:3:DG:H5'	1.90	0.53
3:A:104:ARG:HG2	3:A:121:SER:OG	2.07	0.53
3:A:81:GLN:HA	3:A:81:GLN:HE21	1.73	0.53
3:A:90:PRO:O	3:A:182:ASN:HB3	2.09	0.53
2:C:18:DG:C2'	2:C:19:DT:H72	2.39	0.53
3:A:81:GLN:NE2	3:A:81:GLN:HA	2.24	0.52
3:A:246:VAL:HG23	3:A:254:LYS:HG2	1.90	0.52
3:A:83:VAL:O	3:A:86:ALA:HB3	2.09	0.52
3:A:472:GLN:HG3	3:A:474:ILE:HD12	1.89	0.52
2:C:17:DA:H8	6:C:195:HOH:O	1.93	0.52
3:A:460:LEU:O	3:A:463:PHE:HB3	2.11	0.51
3:A:201:LEU:O	3:A:202:ALA:C	2.46	0.51
3:A:270:ILE:CG1	3:A:279:LEU:HD23	2.40	0.51
2:C:18:DG:H2'	2:C:19:DT:H72	1.93	0.51
3:A:133:GLU:O	3:A:137:PHE:HA	2.10	0.51
3:A:437:ASP:OD2	3:A:440:ARG:HA	2.11	0.51
3:A:275:GLY:CA	3:A:277:ILE:HG23	2.40	0.51
3:A:270:ILE:HD11	3:A:279:LEU:HD21	1.93	0.50
3:A:24:ASP:OD1	3:A:26:ARG:HB2	2.10	0.50
3:A:466:ALA:O	3:A:467:LYS:O	2.30	0.50
3:A:247:VAL:HG12	3:A:248:ASP:N	2.25	0.50
3:A:280:ASN:HB3	3:A:306:VAL:HG21	1.93	0.50
3:A:98:THR:OG1	3:A:127:HIS:ND1	2.45	0.50
3:A:189:ARG:HG3	6:A:579:HOH:O	2.13	0.49
3:A:427:MET:O	3:A:431:ARG:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:191:ALA:O	3:A:193:ILE:N	2.46	0.49
3:A:116:SER:O	3:A:119:ASP:HB2	2.12	0.49
3:A:314:ARG:O	3:A:318:ILE:HG13	2.13	0.49
3:A:401:GLU:O	3:A:402:CYS:C	2.51	0.48
3:A:275:GLY:O	3:A:276:ASN:C	2.48	0.48
1:B:19:DA:H2'	1:B:20:DG:O4'	2.13	0.48
3:A:469:LEU:HA	3:A:474:ILE:HD12	1.95	0.48
1:B:1:DG:H2"	1:B:2:DA:OP2	2.13	0.48
3:A:163:GLY:HA2	3:A:166:LEU:HD12	1.95	0.48
3:A:272:LEU:O	3:A:276:ASN:HA	2.14	0.48
3:A:280:ASN:HB3	3:A:306:VAL:CG2	2.44	0.48
3:A:144:HIS:ND1	6:A:497:HOH:O	2.35	0.48
3:A:288:ASN:N	3:A:289:PRO:HD3	2.29	0.48
2:C:20:DC:O5'	2:C:20:DC:H2'	2.13	0.47
3:A:95:ILE:O	3:A:129:VAL:HA	2.14	0.47
3:A:324:ARG:HG3	3:A:324:ARG:O	2.13	0.47
3:A:476:ILE:CG1	3:A:477:GLY:N	2.77	0.47
3:A:111:LEU:HD13	3:A:123:GLY:HA2	1.96	0.47
1:B:6:DG:H2"	1:B:7:DT:O5'	2.14	0.47
3:A:246:VAL:HG23	3:A:254:LYS:CG	2.45	0.47
3:A:153:ASP:O	3:A:156:ASP:HB2	2.15	0.47
3:A:285:GLU:HG3	3:A:297:LYS:HB2	1.97	0.47
3:A:200:LYS:HD2	3:A:200:LYS:HA	1.75	0.47
3:A:200:LYS:NZ	3:A:205:GLU:HB3	2.30	0.47
1:B:20:DG:N3	3:A:323:TRP:HH2	2.13	0.47
3:A:405:LEU:HD21	3:A:428:ALA:HB3	1.97	0.47
3:A:241:ILE:CD1	3:A:261:ALA:HB2	2.45	0.47
3:A:430:ALA:HA	3:A:449:LEU:HD23	1.96	0.46
3:A:30:ARG:HG2	6:A:488:HOH:O	2.15	0.46
1:B:2:DA:H2"	1:B:3:DC:OP2	2.14	0.46
3:A:476:ILE:HG12	3:A:477:GLY:N	2.30	0.46
3:A:114:LEU:HD12	3:A:122:ARG:HA	1.98	0.46
3:A:181:SER:HA	6:A:626:HOH:O	2.14	0.46
3:A:474:ILE:HG22	3:A:475:LYS:N	2.31	0.46
3:A:164:LYS:CG	3:A:165:TRP:N	2.79	0.46
3:A:467:LYS:O	3:A:470:MET:HG2	2.15	0.46
2:C:18:DG:C2'	2:C:19:DT:C7	2.95	0.45
2:C:14:DA:C2'	2:C:15:DC:H5"	2.45	0.45
3:A:260:LYS:CB	3:A:260:LYS:NZ	2.79	0.45
2:C:11:DT:H2'	2:C:11:DT:H6	1.43	0.45
3:A:418:LYS:O	3:A:420:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:92:LEU:HD23	3:A:133:GLU:HA	1.99	0.45
3:A:288:ASN:N	3:A:289:PRO:CD	2.79	0.45
3:A:270:ILE:HG12	3:A:279:LEU:HD23	1.98	0.45
3:A:275:GLY:HA3	3:A:277:ILE:HG23	1.99	0.45
3:A:241:ILE:HB	3:A:259:ARG:HG2	1.98	0.45
3:A:70:SER:O	3:A:73:ALA:HB3	2.16	0.45
2:C:18:DG:H2"	2:C:19:DT:C7	2.47	0.45
3:A:50:SER:O	3:A:51:GLU:C	2.55	0.44
2:C:4:DA:H2"	2:C:5:DC:O5'	2.18	0.44
3:A:398:THR:H	3:A:401:GLU:HG3	1.82	0.44
3:A:164:LYS:O	3:A:165:TRP:C	2.53	0.44
3:A:16:VAL:HA	3:A:81:GLN:HG2	1.99	0.44
3:A:30:ARG:HD3	3:A:30:ARG:HA	1.78	0.44
3:A:300:LEU:C	3:A:301:LEU:HD23	2.37	0.44
3:A:80:MET:HE1	3:A:175:ARG:HD3	1.98	0.44
3:A:304:GLU:HA	3:A:305:PRO:HD2	1.74	0.44
3:A:399:PRO:O	3:A:403:GLN:HB2	2.17	0.44
1:B:12:DA:OP2	3:A:440:ARG:NH1	2.44	0.44
3:A:60:ALA:O	3:A:64:ILE:HG23	2.17	0.44
1:B:1:DG:H5'	1:B:1:DG:C8	2.53	0.44
3:A:153:ASP:OD1	3:A:154:PRO:HD2	2.18	0.44
3:A:246:VAL:CG2	3:A:254:LYS:HG3	2.48	0.43
2:C:10:DA:H2'	2:C:11:DT:H71	2.00	0.43
3:A:228:LEU:HD12	3:A:299:LEU:HD11	2.00	0.43
3:A:398:THR:H	3:A:401:GLU:CG	2.31	0.43
3:A:264:SER:O	3:A:284:ALA:HA	2.18	0.43
3:A:38:LEU:HA	3:A:38:LEU:HD23	1.79	0.43
2:C:15:DC:H5'	2:C:15:DC:C6	2.53	0.43
3:A:19:SER:O	3:A:20:ALA:C	2.52	0.43
3:A:31:LEU:HD12	3:A:31:LEU:C	2.38	0.43
3:A:437:ASP:CG	3:A:440:ARG:HA	2.39	0.43
3:A:468:ASP:OD1	3:A:472:GLN:OE1	2.37	0.43
3:A:8:ARG:NH1	3:A:401:GLU:OE2	2.50	0.43
3:A:467:LYS:O	3:A:469:LEU:N	2.52	0.43
3:A:423:GLN:O	3:A:424:TRP:C	2.55	0.43
3:A:239:ILE:HD11	3:A:296:LEU:CD1	2.49	0.43
3:A:28:THR:O	3:A:31:LEU:HB3	2.19	0.43
3:A:272:LEU:HB2	3:A:277:ILE:HG12	2.00	0.43
3:A:467:LYS:O	3:A:468:ASP:C	2.56	0.43
3:A:270:ILE:HD11	3:A:279:LEU:CD2	2.48	0.43
3:A:197:LEU:HA	3:A:197:LEU:HD23	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:114:LEU:HD12	3:A:122:ARG:CA	2.49	0.42
3:A:273:LYS:CG	3:A:274:GLN:N	2.82	0.42
3:A:469:LEU:O	3:A:474:ILE:HD12	2.19	0.42
3:A:200:LYS:HZ1	3:A:205:GLU:HB3	1.84	0.42
3:A:404:LEU:O	3:A:405:LEU:C	2.56	0.42
3:A:272:LEU:HA	3:A:272:LEU:HD23	1.71	0.42
3:A:12:TRP:CE2	3:A:362:ARG:HD2	2.55	0.42
3:A:188:ASP:HA	3:A:319:TYR:OH	2.18	0.42
2:C:2:DT:H72	3:A:263:LEU:CD2	2.49	0.42
3:A:79:ALA:O	3:A:82:THR:N	2.52	0.42
3:A:243:GLN:NE2	3:A:255:ASN:OD1	2.44	0.42
3:A:125:TRP:HB2	3:A:148:TRP:CE2	2.55	0.42
3:A:194:HIS:O	3:A:198:GLN:HB2	2.19	0.41
3:A:197:LEU:O	3:A:198:GLN:C	2.58	0.41
3:A:22:LEU:HD12	3:A:28:THR:N	2.35	0.41
3:A:246:VAL:HG22	3:A:254:LYS:O	2.21	0.41
3:A:194:HIS:O	3:A:195:ALA:C	2.54	0.41
2:C:14:DA:C2'	2:C:15:DC:C5'	2.98	0.41
1:B:12:DA:C2	2:C:10:DA:C2	3.08	0.41
3:A:87:GLN:HA	3:A:179:MET:SD	2.60	0.41
3:A:320:THR:O	3:A:320:THR:HG22	2.21	0.41
3:A:173:ARG:HA	3:A:180:MET:HG3	2.03	0.41
3:A:397:LEU:HB3	3:A:401:GLU:HG3	2.01	0.41
3:A:267:SER:HB2	3:A:306:VAL:HB	2.03	0.41
2:C:16:DA:H2"	6:C:195:HOH:O	2.21	0.41
3:A:247:VAL:CG1	3:A:248:ASP:N	2.83	0.41
1:B:13:DA:H2"	1:B:14:DG:C8	2.56	0.41
3:A:291:LYS:HB2	3:A:291:LYS:HE2	1.72	0.41
1:B:2:DA:H1'	1:B:3:DC:H5'	2.03	0.41
3:A:111:LEU:HB3	3:A:123:GLY:HA2	2.03	0.40
3:A:469:LEU:N	3:A:469:LEU:HD23	2.29	0.40
3:A:80:MET:CE	3:A:175:ARG:HD3	2.50	0.40
3:A:224:LEU:O	3:A:225:TYR:C	2.58	0.40
3:A:196:TYR:O	3:A:197:LEU:C	2.60	0.40
2:C:5:DC:O3'	3:A:445:SER:HB3	2.21	0.40
3:A:114:LEU:HD11	3:A:122:ARG:C	2.41	0.40
3:A:263:LEU:HD12	3:A:263:LEU:N	2.36	0.40
3:A:27:ARG:HD2	3:A:27:ARG:HH11	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	452/481 (94%)	423 (94%)	23 (5%)	6 (1%)	15 15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	274	GLN
3	A	192	ASP
3	A	468	ASP
3	A	467	LYS
3	A	473	GLY
3	A	292	GLY

5.3.2 Protein sidechains

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	367/393 (93%)	324 (88%)	43 (12%)	7 7

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	SER
3	A	30	ARG
3	A	44	LYS
3	A	54	LYS
3	A	72	GLU

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Mol	Chain	Res	Type
3	A	80	MET
3	A	88	GLU
3	A	95	ILE
3	A	116	SER
3	A	118	GLN
3	A	119	ASP
3	A	131	LEU
3	A	132	LEU
3	A	136	THR
3	A	159	GLU
3	A	166	LEU
3	A	178	SER
3	A	187	CYS
3	A	188	ASP
3	A	206	ARG
3	A	229	LYS
3	A	240	SER
3	A	252	LYS
3	A	254	LYS
3	A	264	SER
3	A	270	ILE
3	A	273	LYS
3	A	274	GLN
3	A	277	ILE
3	A	279	LEU
3	A	291	LYS
3	A	293	GLU
3	A	297	LYS
3	A	301	LEU
3	A	343	MET
3	A	367	ARG
3	A	392	SER
3	A	395	THR
3	A	410	LYS
3	A	413	ARG
3	A	436	MET
3	A	475	LYS
3	A	476	ILE

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

Mol	Chain	Res	Type
3	A	81	GLN
3	A	87	GLN

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

Of 2 ligands modelled in this entry, 2 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

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	B	20/20 (100%)	-0.19	2 (10%) 9 14	33, 46, 84, 97	0
2	C	20/20 (100%)	-0.06	1 (5%) 32 41	34, 56, 78, 90	0
3	A	455/481 (94%)	0.03	27 (5%) 26 34	28, 47, 90, 100	0
All	All	495/521 (95%)	0.02	30 (6%) 25 33	28, 47, 90, 100	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	474	ILE	5.2
3	A	290	PRO	4.7
3	A	292	GLY	4.0
2	C	20	DC	3.7
1	B	1	DG	3.4
3	A	473	GLY	3.1
3	A	472	GLN	3.1
3	A	469	LEU	3.0
3	A	353	VAL	2.9
3	A	372	PRO	2.9
3	A	291	LYS	2.8
1	B	2	DA	2.8
3	A	477	GLY	2.7
3	A	208	VAL	2.6
3	A	209	VAL	2.6
3	A	7	HIS	2.6
3	A	355	ILE	2.5
3	A	415	ARG	2.5
3	A	95	ILE	2.5
3	A	250	ARG	2.4
3	A	186	VAL	2.4
3	A	354	SER	2.4
3	A	5	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	187	CYS	2.3
3	A	93	LEU	2.3
3	A	470	MET	2.3
3	A	131	LEU	2.3
3	A	130	LEU	2.2
3	A	117	ILE	2.1
3	A	300	LEU	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 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, 95^{th} 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	MN	A	478	1/1	1.00	0.06	-2.73	42,42,42,42	0
5	MG	A	479	1/1	0.87	0.05	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.