Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:15 AM GMT

PDB ID	:	3HOT
Title	:	Crystal structure of the Mos1 mariner paired end complex with Mn
Authors	:	Richardson, J.M.; Walkinshaw, M.D.
Deposited on	:	2009-06-03
Resolution	:	3.25 Å(reported)

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

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

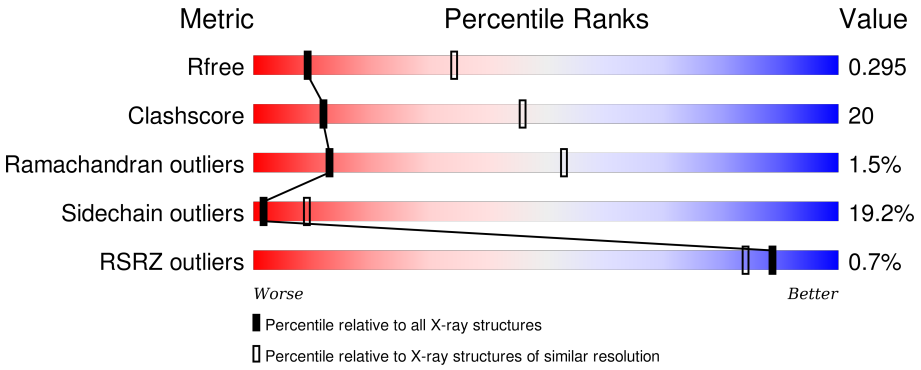
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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 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	345	52% 37% 9% .
1	B	345	% 55% 34% 9% .
2	C	25	32% 48% 20%
2	E	25	40% 40% 20%
2	G	25	4% . 52% 44%

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Mol	Chain	Length	Quality of chain
3	D	28	21% 39% 39%
3	F	28	7% 50% 43%
3	H	28	4% 7% 46% 46%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8915 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 Transposable element mariner, complete cds.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2822	1789	512	511	10			
1	B	338	Total	C	N	O	S	0	0	0
			2821	1789	511	511	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	THR	LYS	SEE REMARK 999	UNP Q7JQ07
A	164	ASN	SER	SEE REMARK 999	UNP Q7JQ07
A	210	PRO	ARG	SEE REMARK 999	UNP Q7JQ07
A	216	ALA	THR	ENGINEERED	UNP Q7JQ07
A	344	PHE	LEU	SEE REMARK 999	UNP Q7JQ07
B	45	THR	LYS	SEE REMARK 999	UNP Q7JQ07
B	164	ASN	SER	SEE REMARK 999	UNP Q7JQ07
B	210	PRO	ARG	SEE REMARK 999	UNP Q7JQ07
B	216	ALA	THR	ENGINEERED	UNP Q7JQ07
B	344	PHE	LEU	SEE REMARK 999	UNP Q7JQ07

- Molecule 2 is a DNA chain called Mos1 NTS inverted repeat DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	25	Total	C	I	N	O	P	0	0	0
			520	247	1	94	153	25			
2	E	25	Total	C	I	N	O	P	0	0	0
			520	247	1	94	153	25			
2	G	25	Total	C	I	N	O	P	0	0	0
			520	247	1	94	153	25			

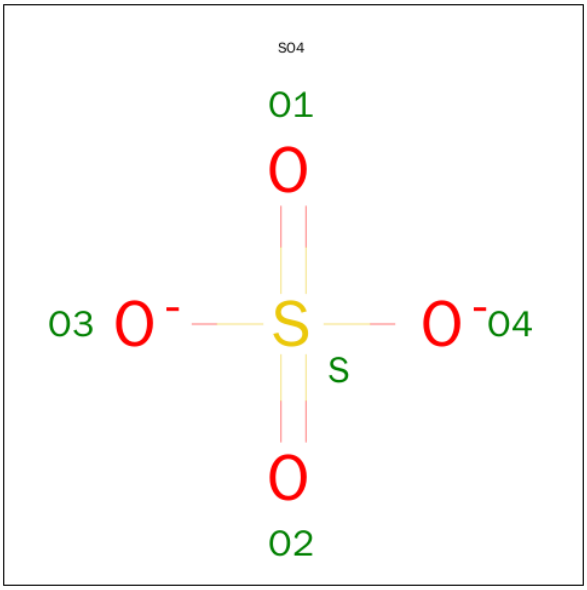
- Molecule 3 is a DNA chain called Mos1 TS inverted repeat DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			
3	F	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			
3	H	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			

- 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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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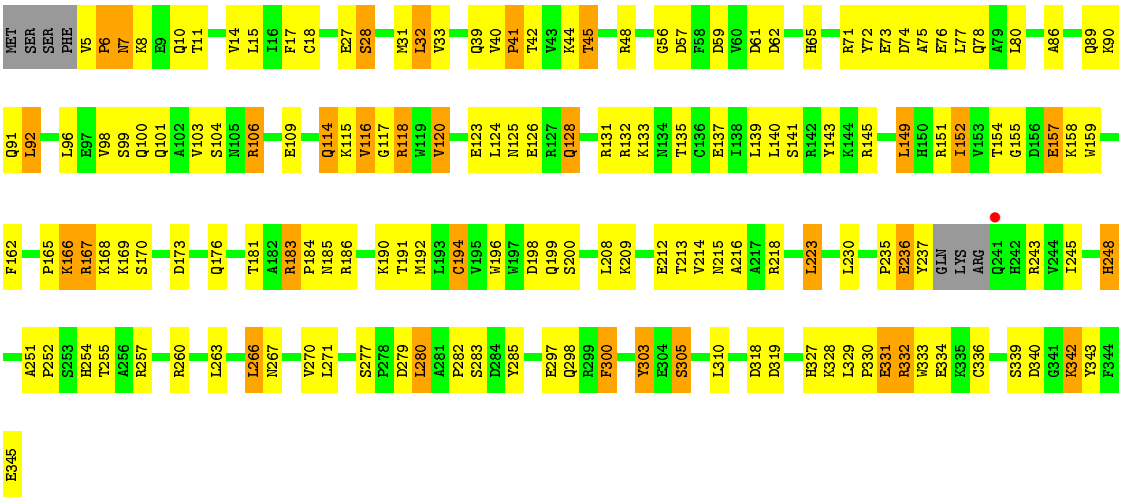
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		

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.

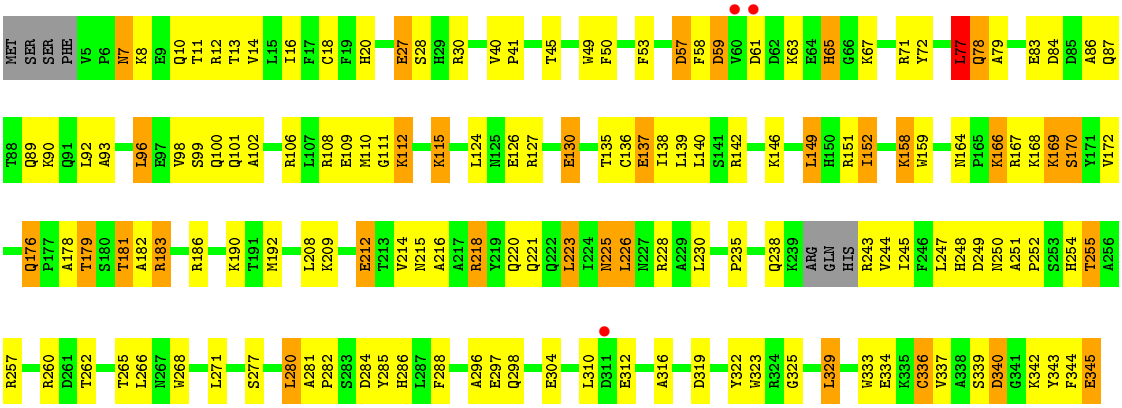
- Molecule 1: Transposable element mariner, complete cds

Chain A:



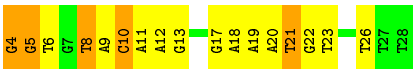
- Molecule 1: Transposable element mariner, complete cds

Chain B:



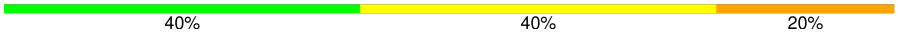
- Molecule 2: Mos1 NTS inverted repeat DNA

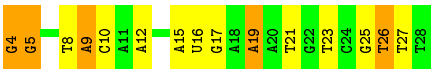
Chain C:



• Molecule 2: Mos1 NTS inverted repeat DNA

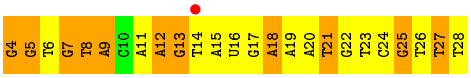
Chain E:





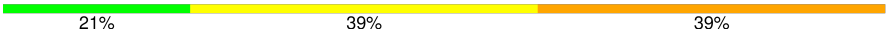
• Molecule 2: Mos1 NTS inverted repeat DNA

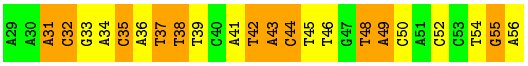
Chain G:



• Molecule 3: Mos1 TS inverted repeat DNA

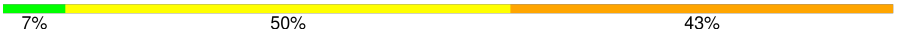
Chain D:





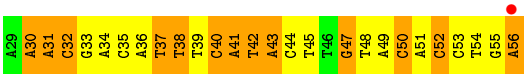
• Molecule 3: Mos1 TS inverted repeat DNA

Chain F:



• Molecule 3: Mos1 TS inverted repeat DNA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.29Å 84.99Å 132.12Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	38.87 – 3.25 38.86 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.2 (38.87-3.25) 93.2 (38.86-3.25)	Depositor EDS
R_{merge}	0.98	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.248 , 0.304 0.245 , 0.295	Depositor DCC
R_{free} test set	1970 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	2 of 38940 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: MN, 5IU, 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	0.58	0/2896	0.70	0/3908
1	B	0.59	2/2894 (0.1%)	0.68	1/3904 (0.0%)
2	C	0.96	1/560 (0.2%)	1.88	20/860 (2.3%)
2	E	1.00	1/560 (0.2%)	2.08	18/860 (2.1%)
2	G	0.91	1/560 (0.2%)	1.69	13/860 (1.5%)
3	D	0.91	0/634	1.86	27/975 (2.8%)
3	F	1.04	0/634	1.94	26/975 (2.7%)
3	H	0.83	0/634	1.74	24/975 (2.5%)
All	All	0.74	5/9372 (0.1%)	1.31	129/13317 (1.0%)

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
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	DG	OP3-P	-10.45	1.48	1.61
2	E	4	DG	OP3-P	-9.49	1.49	1.61
2	C	4	DG	OP3-P	-9.30	1.50	1.61
1	B	126	GLU	CD-OE2	7.98	1.34	1.25
1	B	345	GLU	CG-CD	5.06	1.59	1.51

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	DG	OP1-P-OP2	-22.35	86.07	119.60
2	E	4	DG	O5'-P-OP2	-15.18	92.04	105.70
2	C	13	DG	O4'-C4'-C3'	-12.75	98.35	106.00
3	F	48	DT	O4'-C4'-C3'	-10.11	99.93	106.00
2	E	25	DG	O4'-C1'-N9	10.08	115.06	108.00
3	F	53	DC	O4'-C1'-N1	9.81	114.87	108.00
3	H	42	DT	O4'-C1'-N1	9.61	114.72	108.00
3	F	42	DT	P-O3'-C3'	9.41	131.00	119.70
2	G	21	DT	O4'-C1'-N1	9.38	114.56	108.00
3	F	55	DG	O4'-C1'-N9	-9.36	101.44	108.00
3	D	44	DC	O4'-C4'-C3'	-8.92	100.65	106.00
2	C	4	DG	OP1-P-OP2	-8.87	106.30	119.60
2	C	17	DG	O4'-C1'-N9	8.58	114.01	108.00
2	G	4	DG	OP1-P-OP2	-8.48	106.88	119.60
3	F	31	DA	P-O3'-C3'	8.46	129.85	119.70
3	F	31	DA	O4'-C4'-C3'	-8.17	101.10	106.00
3	H	45	DT	O4'-C1'-N1	8.01	113.61	108.00
3	D	33	DG	O4'-C4'-C3'	-7.83	101.30	106.00
2	C	12	DA	O4'-C4'-C3'	-7.81	101.32	106.00
2	C	13	DG	O4'-C1'-N9	7.79	113.46	108.00
3	F	35	DC	O4'-C1'-N1	7.77	113.44	108.00
3	D	34	DA	O4'-C1'-N9	7.75	113.43	108.00
3	F	40	DC	P-O3'-C3'	7.70	128.94	119.70
3	F	38	DT	P-O3'-C3'	7.66	128.89	119.70
3	D	35	DC	O4'-C1'-N1	7.63	113.34	108.00
2	C	8	DT	P-O3'-C3'	7.61	128.83	119.70
2	E	25	DG	P-O3'-C3'	7.51	128.72	119.70
2	G	9	DA	O4'-C1'-N9	7.45	113.22	108.00
1	B	77	LEU	CA-CB-CG	7.33	132.16	115.30
3	H	49	DA	O4'-C1'-N9	7.27	113.09	108.00
3	D	32	DC	O4'-C1'-N1	7.25	113.07	108.00
2	E	26	DT	O4'-C1'-N1	7.22	113.06	108.00
3	F	50	DC	C1'-O4'-C4'	-7.19	102.91	110.10
2	E	4	DG	O4'-C1'-N9	-7.16	102.99	108.00
3	D	52	DC	O4'-C1'-N1	7.15	113.01	108.00
2	E	21	DT	C1'-O4'-C4'	-7.14	102.96	110.10
2	G	5	DG	O4'-C1'-N9	7.12	112.99	108.00
2	E	19	DA	O4'-C1'-N9	-7.11	103.03	108.00
3	D	42	DT	P-O3'-C3'	7.06	128.18	119.70
3	H	47	DG	O4'-C1'-N9	7.05	112.94	108.00
2	E	23	DT	O4'-C1'-N1	7.03	112.92	108.00
2	E	5	DG	P-O3'-C3'	6.97	128.06	119.70
3	D	41	DA	P-O3'-C3'	6.96	128.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	38	DT	P-O3'-C3'	6.87	127.94	119.70
3	D	49	DA	O4'-C4'-C3'	-6.87	101.75	104.50
3	F	31	DA	C4'-C3'-C2'	-6.80	96.98	103.10
3	H	50	DC	O4'-C1'-N1	6.78	112.75	108.00
2	C	13	DG	C1'-O4'-C4'	-6.75	103.34	110.10
3	H	37	DT	P-O3'-C3'	6.73	127.78	119.70
3	D	39	DT	P-O3'-C3'	6.62	127.64	119.70
3	D	42	DT	O4'-C4'-C3'	-6.58	101.87	104.50
3	D	38	DT	P-O3'-C3'	6.50	127.50	119.70
3	F	45	DT	C6-C5-C7	-6.45	119.03	122.90
3	D	50	DC	C3'-C2'-C1'	-6.45	94.76	102.50
3	D	54	DT	P-O3'-C3'	6.45	127.44	119.70
3	D	52	DC	P-O3'-C3'	6.44	127.43	119.70
3	F	46	DT	O4'-C1'-N1	6.43	112.50	108.00
3	D	31	DA	O4'-C1'-N9	6.36	112.45	108.00
2	G	8	DT	O4'-C1'-C2'	-6.24	100.91	105.90
2	G	27	DT	C1'-O4'-C4'	-6.20	103.90	110.10
3	H	30	DA	C4'-C3'-C2'	-6.19	97.53	103.10
2	E	4	DG	O4'-C1'-C2'	-6.18	100.96	105.90
3	F	37	DT	P-O3'-C3'	6.15	127.08	119.70
3	H	32	DC	C1'-O4'-C4'	-6.12	103.98	110.10
3	H	47	DG	P-O3'-C3'	6.08	126.99	119.70
3	F	31	DA	O4'-C1'-N9	6.00	112.20	108.00
2	C	26	DT	O4'-C1'-N1	5.99	112.19	108.00
2	G	13	DG	P-O3'-C3'	5.91	126.79	119.70
3	D	48	DT	O4'-C1'-N1	5.88	112.12	108.00
3	F	54	DT	N3-C4-O4	5.86	123.42	119.90
3	F	45	DT	C4-C5-C7	5.86	122.52	119.00
3	H	40	DC	P-O3'-C3'	5.83	126.69	119.70
2	C	23	DT	P-O3'-C3'	5.82	126.68	119.70
3	F	54	DT	C5-C4-O4	-5.78	120.86	124.90
3	F	41	DA	P-O3'-C3'	5.77	126.63	119.70
3	D	38	DT	C5-C4-O4	-5.77	120.86	124.90
3	H	52	DC	P-O3'-C3'	5.77	126.62	119.70
3	D	38	DT	C1'-O4'-C4'	-5.75	104.35	110.10
3	H	44	DC	O4'-C1'-N1	5.67	111.97	108.00
3	H	56	DA	O4'-C1'-N9	5.67	111.97	108.00
2	E	12	DA	P-O3'-C3'	5.64	126.47	119.70
3	D	43	DA	O4'-C1'-N9	-5.64	104.05	108.00
3	D	48	DT	P-O3'-C3'	5.60	126.42	119.70
3	H	44	DC	P-O3'-C3'	5.60	126.42	119.70
3	F	39	DT	O4'-C1'-N1	5.59	111.91	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	32	DC	P-O3'-C3'	5.59	126.41	119.70
3	H	43	DA	O4'-C1'-N9	5.59	111.91	108.00
2	C	8	DT	O4'-C4'-C3'	5.57	109.34	106.00
3	F	42	DT	C6-C5-C7	-5.53	119.58	122.90
2	E	21	DT	C5-C4-O4	-5.53	121.03	124.90
3	H	30	DA	O4'-C1'-N9	5.52	111.86	108.00
2	C	21	DT	C6-C5-C7	-5.50	119.60	122.90
3	F	52	DC	C4'-C3'-C2'	-5.48	98.17	103.10
2	C	4	DG	P-O3'-C3'	5.47	126.26	119.70
3	D	44	DC	C1'-O4'-C4'	-5.46	104.64	110.10
3	D	37	DT	P-O3'-C3'	5.43	126.21	119.70
3	D	50	DC	C1'-O4'-C4'	-5.42	104.68	110.10
2	C	6	DT	P-O3'-C3'	5.41	126.19	119.70
2	G	18	DA	O4'-C1'-N9	5.41	111.78	108.00
3	F	29	DA	P-O3'-C3'	5.40	126.18	119.70
2	C	6	DT	C5-C4-O4	-5.35	121.15	124.90
2	G	7	DG	O4'-C4'-C3'	5.35	109.21	106.00
3	H	45	DT	C1'-O4'-C4'	-5.34	104.75	110.10
3	D	46	DT	C5-C4-O4	-5.34	121.16	124.90
3	D	31	DA	C1'-O4'-C4'	-5.32	104.78	110.10
2	G	12	DA	O4'-C1'-N9	5.32	111.72	108.00
2	E	19	DA	P-O3'-C3'	5.32	126.08	119.70
3	H	31	DA	O4'-C1'-N9	5.31	111.72	108.00
3	D	55	DG	O4'-C1'-N9	-5.29	104.29	108.00
2	G	25	DG	C4'-C3'-C2'	5.25	107.83	103.10
2	C	23	DT	C6-C5-C7	-5.23	119.76	122.90
3	F	35	DC	P-O3'-C3'	5.22	125.97	119.70
2	E	8	DT	N3-C4-O4	5.21	123.03	119.90
2	C	21	DT	C4-C5-C7	5.19	122.12	119.00
2	C	12	DA	C1'-O4'-C4'	-5.18	104.92	110.10
2	C	6	DT	N3-C4-O4	5.18	123.01	119.90
3	F	50	DC	O4'-C1'-C2'	-5.17	101.77	105.90
2	E	10	DC	O4'-C1'-C2'	-5.16	101.78	105.90
3	H	36	DA	O4'-C1'-N9	5.14	111.60	108.00
3	H	35	DC	C1'-O4'-C4'	-5.13	104.97	110.10
2	C	10	DC	O4'-C1'-N1	5.13	111.59	108.00
2	C	5	DG	O4'-C1'-N9	5.11	111.58	108.00
2	G	4	DG	O4'-C1'-N9	5.10	111.57	108.00
3	F	48	DT	N3-C4-O4	5.10	122.96	119.90
3	H	35	DC	O4'-C1'-N1	5.06	111.54	108.00
2	G	27	DT	O4'-C4'-C3'	-5.04	102.48	104.50
3	H	41	DA	O4'-C1'-N9	-5.04	104.47	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	17	DG	O4'-C4'-C3'	-5.02	102.49	104.50
2	E	9	DA	N1-C6-N6	5.02	121.61	118.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LEU	Peptide
1	B	111	GLY	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	2822	0	2754	129	0
1	B	2821	0	2760	116	0
2	C	520	0	282	17	0
2	E	520	0	282	9	0
2	G	520	0	282	28	0
3	D	566	0	318	17	0
3	F	566	0	318	23	0
3	H	566	0	318	24	0
4	A	1	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	A	1	0	0	1	0
6	B	2	0	0	0	0
All	All	8915	0	7314	323	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 20.

All (323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PRO:HG3	1:B:329:LEU:HD21	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:HH21	1:A:106:ARG:HG3	1.14	1.02
1:A:100:GLN:HE22	2:C:9:DA:H62	1.03	0.98
1:A:209:LYS:O	1:A:212:GLU:HB2	1.64	0.98
1:A:139:LEU:HD21	1:A:271:LEU:HD22	1.47	0.96
1:A:183:ARG:HG2	1:A:183:ARG:HH11	1.30	0.96
1:A:282:PRO:HG3	1:A:329:LEU:HD21	1.48	0.92
2:G:4:DG:OP3	2:G:4:DG:H8	1.53	0.91
1:B:106:ARG:O	1:B:110:MET:HG3	1.72	0.89
1:A:71:ARG:HD2	3:D:44:DC:H5'	1.55	0.87
1:B:166:LYS:H	1:B:166:LYS:HD3	1.41	0.85
1:B:40:VAL:HB	1:B:41:PRO:HD2	1.61	0.83
1:A:106:ARG:NH2	1:A:106:ARG:HG3	1.93	0.83
1:A:186:ARG:HD2	3:H:55:DG:H4'	1.60	0.82
3:F:32:DC:H2"	3:F:33:DG:H5'	1.61	0.82
1:A:166:LYS:HZ1	1:A:297:GLU:HG3	1.46	0.81
2:G:24:DC:H2'	2:G:25:DG:C8	2.15	0.81
1:A:143:TYR:HE1	1:A:149:LEU:HD21	1.47	0.80
1:B:100:GLN:HE22	2:E:9:DA:H62	1.30	0.79
2:G:4:DG:OP3	2:G:4:DG:C8	2.35	0.79
2:G:7:DG:H2"	2:G:8:DT:OP2	1.82	0.77
1:B:172:VAL:CG2	1:B:176:GLN:HB3	2.15	0.77
1:B:67:LYS:HD2	3:F:43:DA:OP1	1.84	0.76
1:B:172:VAL:HG21	1:B:176:GLN:HB3	1.70	0.74
1:A:140:LEU:HD21	1:A:334:GLU:HG3	1.71	0.73
3:D:56:DA:H4'	3:D:56:DA:OP1	1.87	0.73
3:H:30:DA:H2'	3:H:31:DA:O4'	1.89	0.72
1:B:158:LYS:HE3	1:B:159:TRP:O	1.90	0.71
1:A:332:ARG:CG	1:A:332:ARG:HH11	2.03	0.71
3:D:37:DT:H2"	3:D:38:DT:OP2	1.89	0.71
1:B:285:TYR:OH	1:B:329:LEU:HD22	1.90	0.70
2:G:4:DG:P	2:G:4:DG:H3'	2.31	0.70
1:B:53:PHE:HA	1:B:57:ASP:HB3	1.74	0.70
1:A:11:THR:HG21	1:A:41:PRO:HG2	1.74	0.69
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.55	0.69
1:A:100:GLN:NE2	2:C:9:DA:H62	1.83	0.69
2:G:20:DA:H2'	2:G:21:DT:O4'	1.92	0.69
2:E:19:DA:OP2	2:E:19:DA:H8	1.76	0.68
3:H:33:DG:H2"	3:H:34:DA:C8	2.29	0.67
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.07	0.67
3:F:31:DA:H2'	3:F:32:DC:C6	2.30	0.66
3:F:31:DA:H2'	3:F:32:DC:H6	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:O	1:B:16:ILE:HG22	1.95	0.66
1:A:168:LYS:HD3	1:A:181:THR:HG21	1.77	0.66
3:D:48:DT:H4'	3:D:49:DA:OP1	1.96	0.66
1:A:300:PHE:HB3	1:A:305:SER:HB3	1.76	0.66
1:A:117:GLY:HA3	1:B:179:THR:O	1.96	0.66
3:D:43:DA:H2"	3:D:44:DC:O5'	1.96	0.65
3:H:42:DT:H2"	3:H:43:DA:C8	2.31	0.65
1:A:140:LEU:HD13	1:A:333:TRP:HE3	1.62	0.65
1:B:282:PRO:HA	1:B:285:TYR:CE1	2.32	0.65
1:A:100:GLN:HE22	2:C:9:DA:N6	1.86	0.65
2:C:8:DT:H2"	2:C:9:DA:O5'	1.97	0.65
2:E:4:DG:N2	2:E:5:DG:C4	2.66	0.65
1:A:106:ARG:CG	1:A:106:ARG:HH21	1.99	0.64
3:H:54:DT:H2"	3:H:55:DG:H5'	1.79	0.64
1:A:158:LYS:HG3	3:F:56:DA:OP2	1.97	0.64
1:B:235:PRO:O	1:B:238:GLN:HG2	1.97	0.64
1:A:176:GLN:O	1:B:115:LYS:HE2	1.97	0.64
1:B:329:LEU:HD12	1:B:333:TRP:CZ2	2.33	0.64
1:B:209:LYS:O	1:B:212:GLU:HB2	1.98	0.64
2:G:15:DA:H2'	2:G:16:5IU:C6	2.28	0.63
1:B:99:SER:O	1:B:102:ALA:HB3	1.98	0.63
2:G:4:DG:OP3	2:G:4:DG:H3'	1.98	0.63
1:B:257:ARG:HH11	1:B:260:ARG:HH12	1.44	0.63
3:H:51:DA:H2"	3:H:52:DC:O5'	1.99	0.62
1:B:257:ARG:HD2	1:B:260:ARG:NH1	2.14	0.62
1:B:27:GLU:HG3	1:B:30:ARG:HH21	1.64	0.62
1:A:151:ARG:HD3	1:A:243:ARG:O	2.00	0.62
1:B:7:ASN:HD21	1:B:10:GLN:H	1.48	0.62
1:A:282:PRO:CG	1:A:329:LEU:HD21	2.26	0.61
1:B:65:HIS:H	1:B:65:HIS:CD2	2.17	0.61
1:A:329:LEU:HD12	1:A:333:TRP:CZ2	2.35	0.61
3:D:42:DT:H2'	3:D:43:DA:C8	2.35	0.61
3:H:31:DA:N6	3:H:32:DC:N4	2.49	0.61
1:B:149:LEU:HA	1:B:152:ILE:HG22	1.82	0.61
1:B:11:THR:HG21	1:B:41:PRO:HG3	1.81	0.61
1:A:282:PRO:HG3	1:A:329:LEU:CD2	2.26	0.61
1:A:208:LEU:HD21	1:A:214:VAL:HG23	1.82	0.61
1:A:245:ILE:HG22	1:A:271:LEU:HG	1.82	0.60
2:G:5:DG:H2"	2:G:6:DT:H5'	1.82	0.60
3:H:33:DG:H2"	3:H:34:DA:H8	1.65	0.60
1:B:78:GLN:HE21	1:B:78:GLN:C	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:43:DA:H2"	3:D:44:DC:O4'	2.02	0.60
1:B:208:LEU:HB3	1:B:212:GLU:HB3	1.84	0.60
2:G:12:DA:H2"	2:G:13:DG:OP2	2.01	0.60
1:B:251:ALA:O	1:B:255:THR:HB	2.01	0.60
1:A:89:GLN:HA	1:A:92:LEU:HD12	1.84	0.60
1:B:221:GLN:O	1:B:225:ASN:ND2	2.35	0.59
3:D:44:DC:H2'	3:D:45:DT:C6	2.37	0.59
1:B:257:ARG:HD2	1:B:260:ARG:HH12	1.65	0.59
3:D:31:DA:H2"	3:D:32:DC:O5'	2.02	0.59
1:B:166:LYS:HD2	1:B:297:GLU:HB2	1.85	0.59
1:B:159:TRP:CE3	1:B:190:LYS:HD2	2.38	0.58
1:B:304:GLU:HA	1:B:304:GLU:OE2	2.04	0.58
3:F:52:DC:H2'	3:F:53:DC:C6	2.37	0.58
2:G:13:DG:H2"	2:G:14:DT:OP2	2.03	0.57
3:F:52:DC:H2"	3:F:53:DC:O5'	2.04	0.57
1:B:89:GLN:HA	1:B:92:LEU:HD12	1.84	0.57
1:B:99:SER:HB2	3:F:45:DT:OP2	2.05	0.57
3:D:44:DC:H2'	3:D:45:DT:H6	1.70	0.57
3:F:47:DG:C2	3:F:48:DT:H1'	2.39	0.57
1:B:245:ILE:CG2	1:B:271:LEU:HG	2.35	0.57
1:B:124:LEU:HG	1:B:343:TYR:CE1	2.40	0.56
1:B:124:LEU:HG	1:B:343:TYR:HE1	1.70	0.56
2:G:6:DT:H2"	2:G:7:DG:C8	2.40	0.56
1:B:284:ASP:HA	1:B:288:PHE:HD2	1.71	0.56
2:E:4:DG:C8	2:E:4:DG:H5"	2.41	0.56
1:B:223:LEU:O	1:B:226:LEU:HB3	2.05	0.56
1:B:18:CYS:HB3	1:B:28:SER:OG	2.06	0.55
1:B:214:VAL:O	1:B:214:VAL:HG13	2.06	0.55
1:B:285:TYR:OH	1:B:329:LEU:CD2	2.54	0.55
1:B:172:VAL:HG22	1:B:176:GLN:HB3	1.88	0.55
3:F:29:DA:H2"	3:F:30:DA:OP2	2.07	0.55
1:A:101:GLN:HG2	2:C:10:DC:N4	2.21	0.55
1:A:106:ARG:CG	1:A:106:ARG:NH2	2.64	0.55
1:A:339:SER:HB3	1:A:342:LYS:CB	2.37	0.55
2:C:21:DT:H2"	2:C:22:DG:H8	1.72	0.54
1:A:208:LEU:HB3	1:A:212:GLU:HB3	1.89	0.54
1:A:32:LEU:HG	1:A:40:VAL:HG21	1.89	0.54
2:G:4:DG:P	2:G:4:DG:H8	2.30	0.54
1:B:7:ASN:ND2	1:B:10:GLN:H	2.04	0.54
1:B:230:LEU:HD21	1:B:244:VAL:HG21	1.89	0.54
1:B:339:SER:O	1:B:340:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:HA	1:B:260:ARG:HH11	1.72	0.54
2:G:18:DA:OP2	2:G:18:DA:H8	1.91	0.54
1:A:166:LYS:O	1:A:166:LYS:HE2	2.09	0.53
1:B:215:ASN:O	1:B:216:ALA:C	2.47	0.53
1:A:14:VAL:O	1:A:17:PHE:HB3	2.09	0.53
1:A:184:PRO:HG2	3:H:56:DA:H61	1.73	0.53
2:G:25:DG:H2'	2:G:26:DT:O4'	2.09	0.53
1:A:251:ALA:HB1	1:A:252:PRO:HD2	1.91	0.53
3:F:56:DA:OP1	3:F:56:DA:H4'	2.09	0.52
1:A:116:VAL:HG23	3:F:52:DC:H5'	1.92	0.52
1:A:248:HIS:CE1	1:A:254:HIS:HB3	2.43	0.52
1:B:249:ASP:O	1:B:251:ALA:N	2.39	0.52
1:B:282:PRO:HA	1:B:285:TYR:CZ	2.44	0.52
1:A:18:CYS:HB3	1:A:28:SER:OG	2.10	0.52
1:A:236:GLU:N	1:A:236:GLU:OE2	2.43	0.52
1:A:118:ARG:HH21	1:A:345:GLU:HG2	1.75	0.52
1:A:328:LYS:O	1:A:332:ARG:HB2	2.09	0.51
1:A:8:LYS:HE2	1:A:41:PRO:HD3	1.92	0.51
1:B:245:ILE:HG22	1:B:271:LEU:HG	1.92	0.51
1:B:93:ALA:HB1	1:B:98:VAL:O	2.10	0.51
3:D:56:DA:O3'	3:H:54:DT:H5"	2.11	0.51
1:A:27:GLU:O	1:A:31:MET:HG2	2.10	0.51
2:G:21:DT:H2"	2:G:22:DG:H5'	1.92	0.51
1:B:225:ASN:HD22	1:B:225:ASN:N	2.08	0.51
1:A:72:TYR:CE1	1:A:106:ARG:NE	2.79	0.51
1:B:296:ALA:C	1:B:298:GLN:H	2.15	0.50
1:A:139:LEU:CD2	1:A:271:LEU:HD22	2.30	0.50
1:B:277:SER:HB3	1:B:280:LEU:HB2	1.92	0.50
1:A:162:PHE:HD1	1:A:190:LYS:HA	1.76	0.50
1:A:245:ILE:CG2	1:A:271:LEU:HG	2.41	0.49
1:A:124:LEU:HG	1:A:343:TYR:CE1	2.47	0.49
1:B:312:GLU:O	1:B:316:ALA:HB2	2.12	0.49
1:A:106:ARG:NH1	3:D:44:DC:OP2	2.45	0.49
2:G:11:DA:H2'	2:G:12:DA:C8	2.47	0.49
1:A:135:THR:HG22	1:A:139:LEU:HD12	1.94	0.49
1:B:252:PRO:O	1:B:255:THR:HG22	2.13	0.49
1:A:165:PRO:HA	1:A:166:LYS:NZ	2.27	0.49
1:B:16:ILE:O	1:B:20:HIS:HD2	1.96	0.49
1:A:117:GLY:HA2	1:B:178:ALA:HB3	1.95	0.49
1:B:65:HIS:HD2	1:B:65:HIS:H	1.56	0.49
1:B:342:LYS:O	1:B:343:TYR:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:DC:H2'	3:D:36:DA:C8	2.47	0.49
1:A:263:LEU:HA	1:A:266:LEU:HD12	1.95	0.49
1:A:62:ASP:HB3	2:C:20:DA:H5"	1.95	0.48
3:F:35:DC:H2"	3:F:36:DA:OP2	2.13	0.48
1:A:140:LEU:HD21	1:A:334:GLU:CG	2.43	0.48
1:A:186:ARG:HB2	3:H:55:DG:H4'	1.95	0.48
2:E:19:DA:OP2	2:E:19:DA:C8	2.62	0.48
1:A:166:LYS:HZ2	1:A:297:GLU:HA	1.78	0.48
2:C:21:DT:H2"	2:C:22:DG:C8	2.47	0.48
1:A:74:ASP:O	1:A:76:GLU:N	2.46	0.48
2:C:4:DG:N2	2:C:5:DG:C6	2.82	0.48
1:A:285:TYR:OH	1:A:329:LEU:HD22	2.13	0.48
1:B:72:TYR:OH	1:B:106:ARG:HG3	2.14	0.48
3:H:37:DT:H2"	3:H:38:DT:OP2	2.12	0.48
1:A:331:GLU:HA	1:A:334:GLU:HB2	1.95	0.48
1:A:208:LEU:CD2	1:A:214:VAL:HG23	2.44	0.48
1:B:186:ARG:HG2	3:H:56:DA:O3'	2.13	0.48
1:B:248:HIS:CD2	1:B:254:HIS:HB3	2.49	0.48
1:A:185:ASN:HA	3:H:55:DG:H21	1.78	0.47
1:A:166:LYS:NZ	1:A:297:GLU:HA	2.29	0.47
1:A:86:ALA:HB2	1:B:170:SER:OG	2.14	0.47
1:B:214:VAL:HA	1:B:218:ARG:HG2	1.96	0.47
2:E:15:DA:H2'	2:E:16:5IU:H6	1.95	0.47
1:B:77:LEU:HD12	1:B:110:MET:SD	2.54	0.47
1:B:249:ASP:C	1:B:251:ALA:H	2.15	0.47
1:B:151:ARG:HD2	1:B:243:ARG:O	2.15	0.47
1:A:332:ARG:CG	1:A:332:ARG:NH1	2.70	0.47
1:B:252:PRO:HA	1:B:255:THR:HG22	1.96	0.47
1:A:157:GLU:HB3	1:A:194:CYS:HB3	1.96	0.47
2:G:27:DT:H2"	2:G:28:DT:O5'	2.14	0.47
2:G:4:DG:H2'	2:G:5:DG:C8	2.50	0.47
3:F:32:DC:H2'	3:F:33:DG:C8	2.49	0.47
1:A:166:LYS:H	1:A:166:LYS:HE2	1.80	0.47
3:F:42:DT:H2"	3:F:43:DA:O5'	2.15	0.47
1:A:7:ASN:HB3	1:A:10:GLN:CD	2.35	0.47
3:F:54:DT:H6	3:F:54:DT:H2'	1.32	0.46
1:B:286:HIS:CD2	1:B:325:GLY:HA3	2.50	0.46
2:C:4:DG:N2	2:C:5:DG:C5	2.83	0.46
1:B:71:ARG:HG3	3:F:44:DC:O5'	2.15	0.46
1:A:168:LYS:CD	1:A:181:THR:HG21	2.42	0.46
1:A:125:ASN:HB2	1:A:128:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TRP:HB3	1:B:53:PHE:CE2	2.51	0.46
1:B:12:ARG:NH2	1:B:59:ASP:H	2.14	0.46
1:A:282:PRO:HA	1:A:285:TYR:CE1	2.51	0.46
1:A:186:ARG:CD	3:H:55:DG:H4'	2.40	0.46
1:A:40:VAL:O	1:A:41:PRO:O	2.34	0.46
1:A:159:TRP:HE3	1:A:191:THR:O	1.99	0.46
2:C:18:DA:C2'	2:C:19:DA:C8	2.98	0.46
1:B:7:ASN:ND2	1:B:10:GLN:OE1	2.49	0.46
1:A:183:ARG:NH1	1:A:183:ARG:CG	2.72	0.45
1:B:53:PHE:CD1	1:B:57:ASP:HB3	2.51	0.45
1:A:303:TYR:CD2	1:A:303:TYR:C	2.89	0.45
1:A:198:ASP:C	1:A:198:ASP:OD1	2.53	0.45
3:H:47:DG:H4'	3:H:48:DT:OP1	2.16	0.45
1:A:120:VAL:O	1:B:183:ARG:HB2	2.17	0.45
1:B:215:ASN:O	1:B:218:ARG:N	2.50	0.45
2:C:10:DC:H2"	2:C:11:DA:H5'	1.99	0.45
2:C:20:DA:H2"	2:C:21:DT:H5"	1.98	0.45
1:A:133:LYS:HG3	1:A:340:ASP:HA	1.98	0.45
1:A:339:SER:HB3	1:A:342:LYS:HB3	1.99	0.45
1:A:114:GLN:HA	1:B:170:SER:O	2.17	0.45
1:A:167:ARG:NH1	6:A:346:HOH:O	2.48	0.45
3:F:46:DT:C2'	3:F:47:DG:O5'	2.64	0.44
1:A:215:ASN:H	1:A:218:ARG:HB3	1.80	0.44
1:B:96:LEU:HB3	1:B:98:VAL:HG12	1.98	0.44
1:A:168:LYS:HD3	1:A:181:THR:CG2	2.46	0.44
1:A:120:VAL:HG12	1:B:182:ALA:HA	1.99	0.44
1:A:183:ARG:NH1	1:A:183:ARG:HG2	2.10	0.44
1:B:214:VAL:O	1:B:214:VAL:CG1	2.65	0.44
1:A:165:PRO:HD2	1:A:184:PRO:HB3	1.98	0.44
1:A:339:SER:HB3	1:A:342:LYS:HB2	1.99	0.44
1:A:41:PRO:HB3	1:A:45:THR:HG21	2.00	0.44
1:A:40:VAL:HG22	1:A:41:PRO:HD2	1.99	0.44
2:G:15:DA:H2'	2:G:16:5IU:C5	2.47	0.44
1:B:140:LEU:HD13	1:B:333:TRP:HB2	2.00	0.44
3:F:41:DA:H2"	3:F:42:DT:H71	2.00	0.44
1:B:139:LEU:CD2	1:B:271:LEU:HD22	2.47	0.44
1:A:7:ASN:HB3	1:A:10:GLN:NE2	2.33	0.44
1:B:152:ILE:HD11	1:B:247:LEU:HB3	1.99	0.44
1:A:89:GLN:C	1:A:91:GLN:H	2.21	0.44
1:B:127:ARG:O	1:B:130:GLU:HG3	2.17	0.44
1:A:155:GLY:HA3	1:A:196:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLY:O	1:A:57:ASP:HB3	2.18	0.43
3:H:54:DT:C2'	3:H:55:DG:H5'	2.47	0.43
1:B:172:VAL:HG22	1:B:176:GLN:CB	2.48	0.43
1:B:84:ASP:HB3	1:B:87:GLN:NE2	2.32	0.43
3:D:56:DA:O3'	3:H:54:DT:OP2	2.37	0.43
1:A:327:HIS:O	1:A:330:PRO:CD	2.66	0.43
1:B:288:PHE:HB3	3:D:55:DG:H4'	2.00	0.43
2:G:8:DT:H2"	2:G:9:DA:H8	1.84	0.43
3:H:52:DC:H2'	3:H:53:DC:C6	2.53	0.43
1:B:12:ARG:CZ	1:B:59:ASP:HB3	2.48	0.43
1:A:318:ASP:OD1	1:A:319:ASP:N	2.47	0.43
1:A:277:SER:HB3	1:A:280:LEU:HD23	2.01	0.43
1:A:140:LEU:O	1:A:143:TYR:HB3	2.19	0.43
1:A:99:SER:O	1:A:103:VAL:HG23	2.19	0.43
2:G:4:DG:H2'	2:G:5:DG:O4'	2.18	0.43
1:A:327:HIS:O	1:A:330:PRO:HD2	2.19	0.43
1:A:117:GLY:HA2	1:B:178:ALA:CB	2.49	0.43
1:B:112:LYS:H	1:B:112:LYS:HG2	1.48	0.43
2:G:4:DG:N2	3:H:53:DC:C2	2.87	0.42
1:A:186:ARG:CB	3:H:55:DG:H4'	2.49	0.42
2:C:18:DA:H2"	2:C:19:DA:C8	2.53	0.42
1:B:296:ALA:O	1:B:298:GLN:N	2.53	0.42
2:G:17:DG:C2	3:H:41:DA:C2	3.07	0.42
1:B:10:GLN:O	1:B:14:VAL:HG23	2.20	0.42
1:A:132:ARG:NH2	1:A:279:ASP:OD1	2.53	0.42
1:B:322:TYR:O	1:B:323:TRP:C	2.58	0.42
1:B:220:GLN:NE2	1:B:262:THR:OG1	2.52	0.42
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.19	0.42
1:B:149:LEU:HA	1:B:152:ILE:CG2	2.48	0.42
1:B:244:VAL:HB	1:B:268:TRP:CD1	2.55	0.42
1:A:123:GLU:HG2	1:B:182:ALA:HB3	2.02	0.42
2:G:18:DA:OP2	2:G:18:DA:H2'	2.19	0.42
2:E:27:DT:OP2	2:E:27:DT:H2'	2.19	0.42
1:A:123:GLU:HG2	1:B:182:ALA:CB	2.49	0.42
1:A:132:ARG:NH1	1:A:342:LYS:O	2.53	0.42
1:A:162:PHE:CD1	1:A:190:LYS:HA	2.54	0.42
1:B:284:ASP:HA	1:B:288:PHE:CD2	2.53	0.42
1:A:235:PRO:HB2	1:A:236:GLU:HG3	2.01	0.42
2:C:18:DA:H2"	2:C:19:DA:H8	1.85	0.42
2:C:8:DT:H2'	2:C:9:DA:C8	2.55	0.41
2:E:26:DT:H2'	2:E:27:DT:H72	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HE3	1:B:181:THR:HG23	2.02	0.41
1:B:79:ALA:O	1:B:83:GLU:HG3	2.20	0.41
1:B:136:CYS:O	1:B:137:GLU:C	2.58	0.41
1:B:135:THR:O	1:B:139:LEU:HG	2.20	0.41
1:A:133:LYS:O	1:A:137:GLU:HB2	2.19	0.41
1:A:230:LEU:HD21	1:A:237:TYR:HD2	1.84	0.41
2:G:23:DT:H2"	2:G:24:DC:H5"	2.02	0.41
1:A:165:PRO:HA	1:A:166:LYS:HZ3	1.85	0.41
2:E:4:DG:N2	2:E:5:DG:C5	2.88	0.41
3:D:35:DC:H5"	3:D:35:DC:H6	1.85	0.41
1:A:86:ALA:HB1	1:B:169:LYS:O	2.20	0.41
2:C:18:DA:H2"	2:C:19:DA:OP2	2.18	0.41
1:A:5:VAL:HA	1:A:6:PRO:HD3	1.80	0.41
1:A:116:VAL:CG2	3:F:52:DC:H5'	2.50	0.41
1:A:72:TYR:O	1:A:72:TYR:CG	2.74	0.41
2:G:19:DA:C2	2:G:20:DA:C4	3.09	0.41
1:A:158:LYS:HG2	1:A:159:TRP:N	2.36	0.41
1:A:128:GLN:O	1:A:132:ARG:HG3	2.20	0.41
3:F:40:DC:H2"	3:F:41:DA:C8	2.55	0.41
3:F:45:DT:H2'	3:F:46:DT:C6	2.55	0.41
1:B:225:ASN:HD22	1:B:225:ASN:H	1.66	0.41
1:B:288:PHE:CB	3:D:55:DG:H4'	2.51	0.41
1:B:281:ALA:HA	1:B:282:PRO:HD3	1.81	0.41
2:G:7:DG:H1	3:H:50:DC:H42	1.69	0.41
1:B:209:LYS:HE2	1:B:212:GLU:OE1	2.21	0.40
1:A:257:ARG:HD2	1:A:260:ARG:HH21	1.86	0.40
1:A:149:LEU:O	1:A:152:ILE:HG22	2.21	0.40
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.86	0.40
3:F:48:DT:H2'	3:F:49:DA:C8	2.56	0.40
1:A:215:ASN:O	1:A:216:ALA:C	2.58	0.40
1:B:140:LEU:HD21	1:B:334:GLU:OE2	2.22	0.40
1:B:50:PHE:HA	1:B:53:PHE:HB2	2.03	0.40
3:H:39:DT:H2"	3:H:40:DC:C6	2.56	0.40
1:A:170:SER:HA	1:B:86:ALA:HA	2.03	0.40
1:B:149:LEU:CA	1:B:152:ILE:HG22	2.50	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
1	A	334/345 (97%)	297 (89%)	31 (9%)	6 (2%)	11 49
1	B	334/345 (97%)	285 (85%)	45 (14%)	4 (1%)	16 58
All	All	668/690 (97%)	582 (87%)	76 (11%)	10 (2%)	13 53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	B	250	ASN
1	A	75	ALA
1	A	267	ASN
1	B	58	PHE
1	A	65	HIS
1	A	128	GLN
1	B	319	ASP
1	B	336	CYS
1	A	6	PRO

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
1	A	300/307 (98%)	238 (79%)	62 (21%)	1 7
1	B	300/307 (98%)	247 (82%)	53 (18%)	2 11
All	All	600/614 (98%)	485 (81%)	115 (19%)	2 9

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	15	LEU
1	A	28	SER
1	A	32	LEU
1	A	33	VAL
1	A	39	GLN
1	A	42	THR
1	A	44	LYS
1	A	45	THR
1	A	48	ARG
1	A	59	ASP
1	A	61	ASP
1	A	73	GLU
1	A	77	LEU
1	A	78	GLN
1	A	80	LEU
1	A	90	LYS
1	A	92	LEU
1	A	96	LEU
1	A	98	VAL
1	A	104	SER
1	A	106	ARG
1	A	109	GLU
1	A	114	GLN
1	A	115	LYS
1	A	116	VAL
1	A	118	ARG
1	A	120	VAL
1	A	126	GLU
1	A	131	ARG
1	A	141	SER
1	A	145	ARG
1	A	149	LEU
1	A	152	ILE
1	A	154	THR
1	A	157	GLU
1	A	166	LYS
1	A	167	ARG
1	A	169	LYS
1	A	173	ASP
1	A	183	ARG
1	A	192	MET

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Mol	Chain	Res	Type
1	A	194	CYS
1	A	199	GLN
1	A	200	SER
1	A	213	THR
1	A	223	LEU
1	A	236	GLU
1	A	248	HIS
1	A	255	THR
1	A	270	VAL
1	A	280	LEU
1	A	283	SER
1	A	298	GLN
1	A	300	PHE
1	A	303	TYR
1	A	305	SER
1	A	310	LEU
1	A	331	GLU
1	A	332	ARG
1	A	336	CYS
1	A	342	LYS
1	B	7	ASN
1	B	8	LYS
1	B	27	GLU
1	B	45	THR
1	B	57	ASP
1	B	59	ASP
1	B	61	ASP
1	B	63	LYS
1	B	65	HIS
1	B	77	LEU
1	B	78	GLN
1	B	90	LYS
1	B	96	LEU
1	B	101	GLN
1	B	108	ARG
1	B	109	GLU
1	B	112	LYS
1	B	115	LYS
1	B	130	GLU
1	B	137	GLU
1	B	138	ILE
1	B	142	ARG

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Mol	Chain	Res	Type
1	B	146	LYS
1	B	149	LEU
1	B	152	ILE
1	B	158	LYS
1	B	164	ASN
1	B	166	LYS
1	B	167	ARG
1	B	169	LYS
1	B	170	SER
1	B	176	GLN
1	B	179	THR
1	B	181	THR
1	B	183	ARG
1	B	192	MET
1	B	212	GLU
1	B	218	ARG
1	B	223	LEU
1	B	225	ASN
1	B	226	LEU
1	B	228	ARG
1	B	255	THR
1	B	265	THR
1	B	266	LEU
1	B	280	LEU
1	B	310	LEU
1	B	329	LEU
1	B	336	CYS
1	B	337	VAL
1	B	340	ASP
1	B	344	PHE
1	B	345	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	51	GLN
1	A	100	GLN
1	A	114	GLN
1	A	122	HIS
1	A	164	ASN
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	293	HIS
1	B	7	ASN
1	B	10	GLN
1	B	20	HIS
1	B	39	GLN
1	B	65	HIS
1	B	87	GLN
1	B	91	GLN
1	B	95	GLN
1	B	100	GLN
1	B	101	GLN
1	B	114	GLN
1	B	225	ASN
1	B	227	ASN
1	B	248	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	5IU	C	16	3	12,21,22	1.66	2 (16%)	14,30,33	2.81	3 (21%)
2	5IU	E	16	-	12,21,22	1.39	1 (8%)	14,30,33	2.66	3 (21%)
2	5IU	G	16	3	12,21,22	0.52	0	14,30,33	2.03	3 (21%)

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
2	5IU	C	16	3	-	0/3/21/22	0/2/2/2
2	5IU	E	16	-	-	0/3/21/22	0/2/2/2
2	5IU	G	16	3	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	16	5IU	C6-C5	2.35	1.44	1.38
2	E	16	5IU	C5-I5	3.46	2.18	2.10
2	C	16	5IU	C5-I5	4.38	2.20	2.10

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	16	5IU	C2'-C1'-N1	-2.74	107.48	114.16
2	E	16	5IU	C6-C5-I5	2.01	124.00	118.99
2	C	16	5IU	C6-C5-I5	2.16	124.38	118.99
2	G	16	5IU	O4'-C1'-N1	2.55	112.12	107.72
2	C	16	5IU	O4'-C1'-N1	3.12	113.11	107.72
2	E	16	5IU	O4'-C1'-N1	3.56	113.87	107.72
2	G	16	5IU	C4-N3-C2	6.21	120.61	115.25
2	E	16	5IU	C4-N3-C2	8.62	122.70	115.25
2	C	16	5IU	C4-N3-C2	8.92	122.96	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	16	5IU	1	0
2	G	16	5IU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
5	SO4	B	346	-	4,4,4	0.18	0	6,6,6	0.11	0
5	SO4	D	1	-	4,4,4	0.15	0	6,6,6	0.12	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
5	SO4	B	346	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1	-	-	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

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	A	338/345 (97%)	-0.02	1 (0%) 94 93	23, 48, 67, 86	0
1	B	338/345 (97%)	0.00	3 (0%) 85 80	24, 49, 73, 84	0
2	C	24/25 (96%)	-0.22	0 100 100	32, 46, 65, 75	0
2	E	24/25 (96%)	-0.12	0 100 100	35, 48, 72, 81	0
2	G	24/25 (96%)	0.47	1 (4%) 40 30	3, 53, 95, 112	0
3	D	28/28 (100%)	-0.21	0 100 100	30, 44, 55, 58	0
3	F	28/28 (100%)	-0.19	0 100 100	32, 48, 63, 68	0
3	H	28/28 (100%)	0.42	1 (3%) 46 37	8, 58, 89, 90	0
All	All	832/849 (97%)	-0.00	6 (0%) 89 84	3, 48, 73, 112	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	GLN	3.3
3	H	56	DA	3.1
1	B	311	ASP	2.6
1	B	60	VAL	2.3
1	B	61	ASP	2.2
2	G	14	DT	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	5IU	E	16	20/21	0.89	0.20	-	57,66,91,108	0
2	5IU	C	16	20/21	0.86	0.21	-	58,68,92,108	0
2	5IU	G	16	20/21	0.69	0.36	-	100,118,131,139	0

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
5	SO4	D	1	5/5	0.82	0.30	-	123,123,123,124	0
4	MN	A	1001	1/1	0.94	0.25	-	89,89,89,89	0
5	SO4	B	346	5/5	0.86	0.20	-	129,129,130,130	0

6.5 Other polymers (i)

There are no such residues in this entry.