



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 2XM3 / pdb_00002xm3
Title : Deinococcus radiodurans ISDra2 Transposase Left end DNA complex
Authors : Hickman, A.B.; James, J.A.; Barabas, O.; Pasternak, C.; Ton-Hoang, B.;
Chandler, M.; Sommer, S.; Dyda, F.
Deposited on : 2010-07-22
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

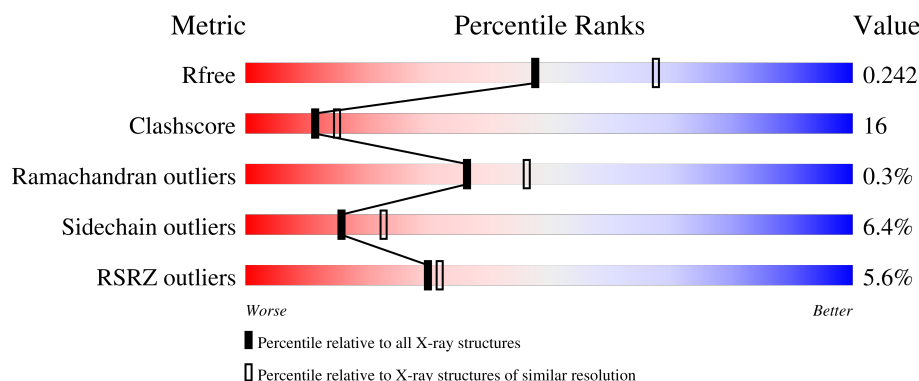
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	140	3% 64% 20% 5% 10%
1	B	140	5% 70% 18% 8%
1	C	140	4% 64% 24% 9%
1	D	140	9% 65% 23% 8%
1	E	140	7% 65% 20% 5% 10%

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Mol	Chain	Length	Quality of chain
1	F	140	
2	G	27	
2	I	27	
2	K	27	
2	M	27	
2	O	27	
2	Q	27	
3	H	5	
3	J	5	
3	L	5	
3	N	5	
3	P	5	
3	R	5	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10596 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 TRANSPOSASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1017	656	176	179	6			
1	B	129	Total	C	N	O	S	0	0	0
			1040	673	179	182	6			
1	C	128	Total	C	N	O	S	0	0	0
			1032	667	178	181	6			
1	D	129	Total	C	N	O	S	0	0	0
			1042	670	182	184	6			
1	E	126	Total	C	N	O	S	0	0	0
			1017	656	176	179	6			
1	F	126	Total	C	N	O	S	0	0	0
			1017	656	176	179	6			

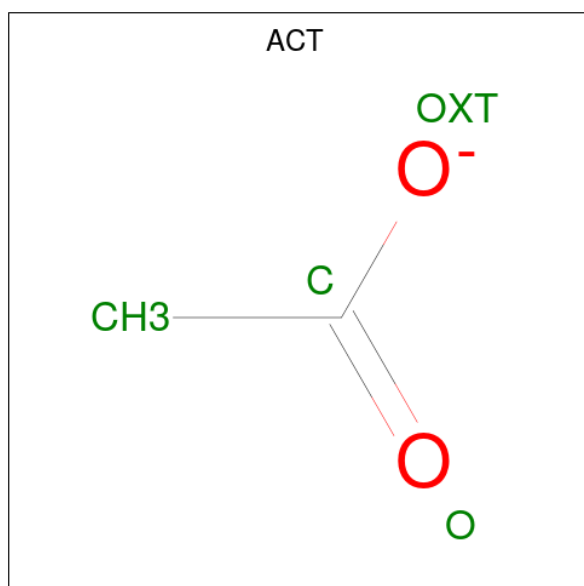
- Molecule 2 is a DNA chain called DRA2 TRANSPOSASE BINDING ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			
2	I	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			
2	K	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			
2	M	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			
2	O	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			
2	Q	27	Total	C	N	O	P	0	0	0
			547	262	98	161	26			

- Molecule 3 is a DNA chain called 5'-D(*TP*TP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			
3	J	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			
3	L	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			
3	N	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			
3	P	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			
3	R	5	Total	C	N	O	P	0	0	0
			100	50	16	30	4			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	2	Total	Mg	0	0
			2	2		
5	K	2	Total	Mg	0	0
			2	2		
5	M	2	Total	Mg	0	0
			2	2		
5	O	1	Total	Mg	0	0
			1	1		
5	Q	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		
6	P	1	Total	C	O	0	0
			6	3	3		

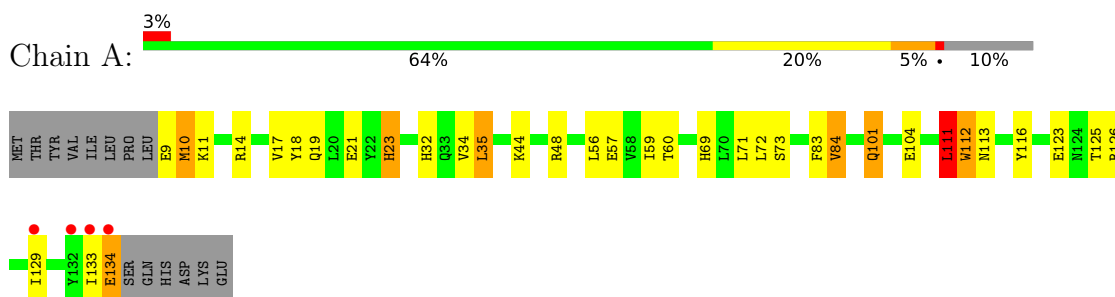
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	58	Total 58	O 58	0	0
7	B	53	Total 53	O 53	0	0
7	C	58	Total 58	O 58	0	0
7	D	43	Total 43	O 43	0	0
7	E	39	Total 39	O 39	0	0
7	F	30	Total 30	O 30	0	0
7	G	35	Total 35	O 35	0	0
7	H	3	Total 3	O 3	0	0
7	I	42	Total 42	O 42	0	0
7	J	8	Total 8	O 8	0	0
7	K	45	Total 45	O 45	0	0
7	L	4	Total 4	O 4	0	0
7	M	29	Total 29	O 29	0	0
7	N	8	Total 8	O 8	0	0
7	O	23	Total 23	O 23	0	0
7	Q	25	Total 25	O 25	0	0
7	R	6	Total 6	O 6	0	0

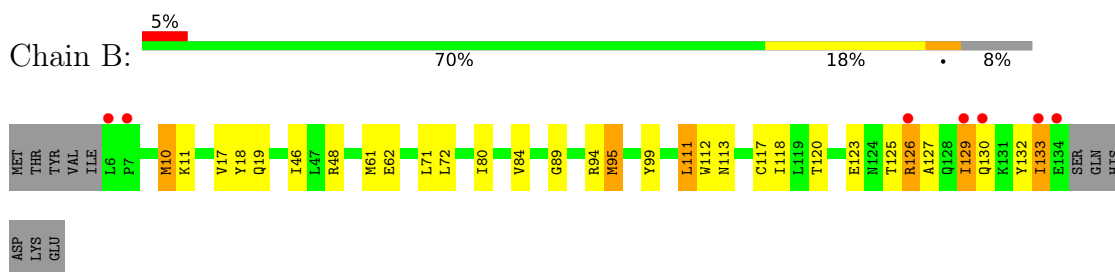
3 Residue-property plots [i](#)

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

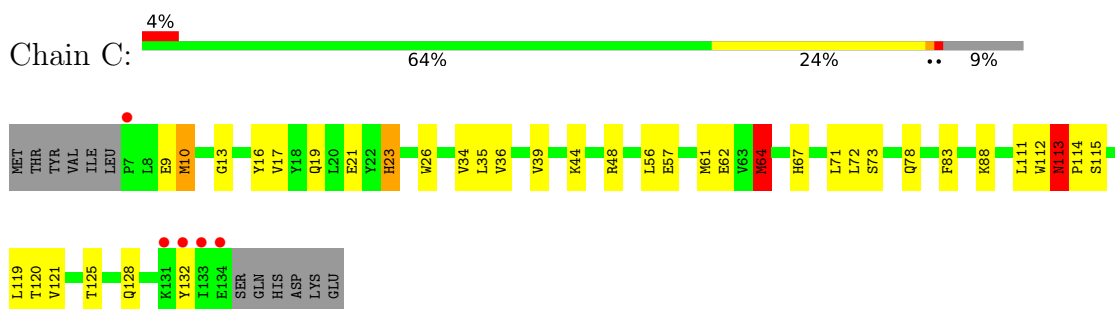
- Molecule 1: TRANSPOSASE



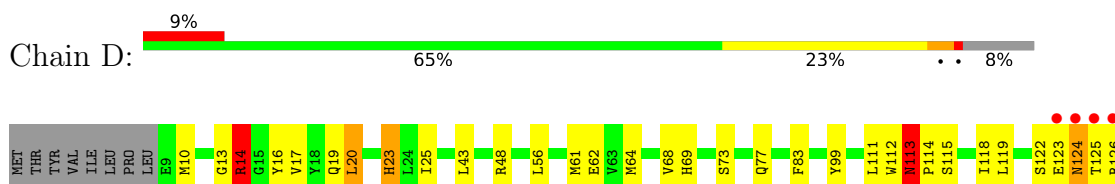
- Molecule 1: TRANSPOSASE

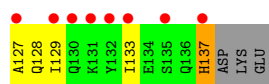


- Molecule 1: TRANSPOSASE



- Molecule 1: TRANSPOSASE

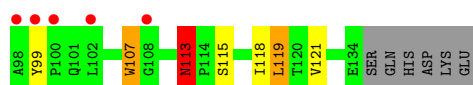




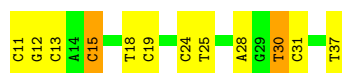
● Molecule 1: TRANSPOSASE



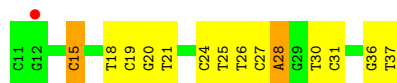
● Molecule 1: TRANSPOSASE



● Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT



● Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT

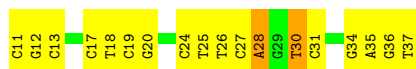


● Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT

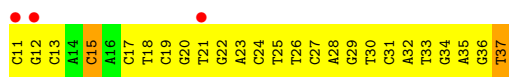


● Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT

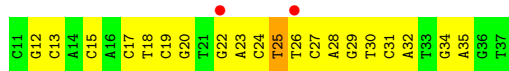




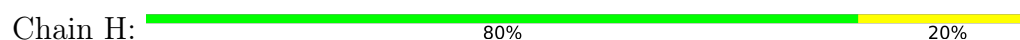
- Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT



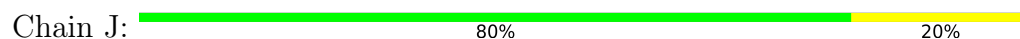
- Molecule 2: DRA2 TRANSPOSASE BINDING ELEMENT



- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'



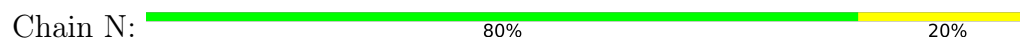
- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'



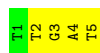
- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'



- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'



- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'



- Molecule 3: 5'-D(*TP*TP*AP*GP*T)-3'

Chain R:

60%

40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 128.38Å 140.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.30) 93.0 (30.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.249 0.211 , 0.242	Depositor DCC
R_{free} test set	1575 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10596	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ACT, GOL, MG

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	0.64	0/1040	1.08	8/1408 (0.6%)
1	B	0.72	1/1064 (0.1%)	1.08	9/1442 (0.6%)
1	C	0.64	0/1056	1.06	8/1430 (0.6%)
1	D	0.63	0/1066	1.08	9/1443 (0.6%)
1	E	0.61	0/1040	1.08	5/1408 (0.4%)
1	F	0.59	0/1040	1.11	6/1408 (0.4%)
2	G	0.40	0/612	0.83	1/942 (0.1%)
2	I	0.41	0/612	0.75	0/942
2	K	0.41	0/612	0.77	0/942
2	M	0.41	0/612	0.82	1/942 (0.1%)
2	O	0.36	0/612	0.75	0/942
2	Q	0.37	0/612	0.75	0/942
3	H	0.37	0/111	0.90	0/170
3	J	0.43	0/111	0.79	0/170
3	L	0.42	0/111	1.09	1/170 (0.6%)
3	N	0.36	0/111	0.90	0/170
3	P	0.38	0/111	0.91	0/170
3	R	0.38	0/111	0.99	1/170 (0.6%)
All	All	0.55	1/10644 (0.0%)	0.97	49/15211 (0.3%)

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
2	G	0	1
2	I	0	2
2	K	0	5
2	M	0	1
2	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Q	0	1
3	P	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	MET	SD-CE	-8.74	1.57	1.79

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	107	TRP	N-CA-C	-9.34	97.47	110.35
1	C	113	ASN	N-CA-C	-7.84	99.87	109.83
1	E	111	LEU	N-CA-C	-7.50	104.25	113.41
1	E	113	ASN	N-CA-C	-7.30	100.56	109.83
3	R	5	DT	C2'-C3'-O3'	-7.29	100.56	111.50
1	A	111	LEU	N-CA-C	-6.95	104.43	113.12
1	F	113	ASN	N-CA-C	-6.91	101.05	109.83
1	D	99	TYR	CA-C-N	6.67	127.20	119.47
1	D	99	TYR	C-N-CA	6.67	127.20	119.47
1	D	113	ASN	N-CA-C	-6.50	101.39	109.64
1	C	111	LEU	N-CA-C	-6.49	105.89	113.88
1	F	18	TYR	N-CA-C	6.44	118.01	108.60
1	A	23	HIS	N-CA-C	-6.41	98.80	109.24
1	D	14	ARG	N-CA-C	6.40	119.06	111.71
1	D	111	LEU	N-CA-C	-6.39	105.61	113.41
1	A	84	VAL	N-CA-C	-6.36	104.55	110.53
1	C	23	HIS	N-CA-C	-6.18	98.44	108.52
1	A	112	TRP	N-CA-C	6.11	120.01	110.17
1	B	113	ASN	N-CA-C	-6.04	101.97	109.64
1	B	112	TRP	N-CA-C	5.96	119.77	110.17
1	A	71	LEU	N-CA-C	-5.94	98.72	108.41
1	E	23	HIS	N-CA-C	-5.84	99.77	109.46
1	D	23	HIS	N-CA-C	-5.74	99.93	109.46
1	F	71	LEU	N-CA-C	-5.73	98.00	108.02
1	F	23	HIS	N-CA-C	-5.67	100.00	109.24
1	E	71	LEU	N-CA-C	-5.64	98.15	108.02
1	A	18	TYR	N-CA-C	5.63	116.82	108.60
1	B	132	TYR	N-CA-C	5.56	119.68	113.01
1	B	18	TYR	N-CA-C	5.53	116.67	108.60
1	C	17	VAL	N-CA-C	-5.52	100.54	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASN	N-CA-C	-5.50	102.66	109.64
1	B	10	MET	N-CA-C	5.45	117.35	109.07
2	M	30	DT	C5'-C4'-C3'	5.44	123.06	114.90
1	B	133	ILE	N-CA-C	-5.39	107.23	112.29
3	L	2	DT	C5'-C4'-O4'	-5.37	101.34	109.40
1	E	112	TRP	N-CA-C	5.30	118.38	109.95
1	A	14	ARG	N-CA-C	5.26	117.42	111.11
1	B	99	TYR	CA-C-N	5.24	125.54	119.47
1	B	99	TYR	C-N-CA	5.24	125.54	119.47
1	C	64	MET	N-CA-C	-5.22	102.57	110.50
1	D	112	TRP	N-CA-C	5.20	118.21	109.95
1	B	111	LEU	N-CA-C	-5.19	105.24	112.45
1	C	112	TRP	N-CA-C	5.18	118.18	109.95
1	F	74	ALA	N-CA-C	5.16	116.13	108.86
1	D	17	VAL	N-CA-C	-5.09	100.88	108.46
2	G	30	DT	C5'-C4'-C3'	5.07	122.51	114.90
1	C	71	LEU	N-CA-C	-5.07	99.15	108.02
1	C	9	GLU	N-CA-C	-5.07	101.70	109.76
1	D	20	LEU	N-CA-C	5.03	116.61	108.41

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	15	DC	Sidechain
2	I	15	DC	Sidechain
2	I	28	DA	Sidechain
2	K	15	DC	Sidechain
2	K	23	DA	Sidechain
2	K	28	DA	Sidechain
2	K	30	DT	Sidechain
2	K	35	DA	Sidechain
2	M	28	DA	Sidechain
2	O	15	DC	Sidechain
2	O	37	DT	Sidechain
3	P	4	DA	Sidechain
2	Q	25	DT	Sidechain

5.2 Too-close contacts

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	1017	0	1033	23	0
1	B	1040	0	1062	21	0
1	C	1032	0	1052	27	0
1	D	1042	0	1053	27	0
1	E	1017	0	1033	25	0
1	F	1017	0	1033	34	0
2	G	547	0	306	13	0
2	I	547	0	306	14	0
2	K	547	0	306	13	0
2	M	547	0	306	26	0
2	O	547	0	306	56	0
2	Q	547	0	306	37	0
3	H	100	0	60	1	0
3	J	100	0	60	1	0
3	L	100	0	60	5	0
3	N	100	0	60	1	0
3	P	100	0	60	6	0
3	R	100	0	60	1	0
4	B	4	0	3	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	I	2	0	0	0	0
5	K	2	0	0	0	0
5	M	2	0	0	0	0
5	O	1	0	0	0	0
5	Q	1	0	0	0	0
6	G	6	0	8	1	0
6	J	6	0	8	2	0
6	L	6	0	8	2	0
6	P	6	0	8	2	0
7	A	58	0	0	2	0
7	B	53	0	0	1	0
7	C	58	0	0	1	0
7	D	43	0	0	0	0
7	E	39	0	0	0	0
7	F	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	35	0	0	0	0
7	H	3	0	0	0	0
7	I	42	0	0	1	0
7	J	8	0	0	0	0
7	K	45	0	0	0	0
7	L	4	0	0	0	0
7	M	29	0	0	0	0
7	N	8	0	0	0	0
7	O	23	0	0	0	0
7	Q	25	0	0	0	0
7	R	6	0	0	0	0
All	All	10596	0	8497	300	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 16.

All (300) 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)
2:O:18:DT:H5'	2:O:18:DT:C6	1.79	1.18
2:O:18:DT:H5'	2:O:18:DT:H6	0.98	1.14
2:M:36:DG:C2'	2:M:37:DT:H5''	1.76	1.13
2:O:17:DC:C2'	2:O:18:DT:H5''	1.78	1.13
2:M:12:DG:H2''	2:M:13:DC:H5''	1.34	1.09
2:Q:24:DC:H2''	2:Q:25:DT:H71	1.32	1.08
2:O:34:DG:H2''	2:O:35:DA:H5'	1.35	1.07
3:P:2:DT:H6	3:P:2:DT:H5'	1.17	1.07
2:O:32:DA:C2'	2:O:33:DT:H5''	1.85	1.06
2:O:21:DT:C2'	2:O:22:DG:H5''	1.89	1.02
2:M:36:DG:H2''	2:M:37:DT:H5''	1.03	1.01
2:Q:24:DC:C2'	2:Q:25:DT:H71	1.92	0.99
2:O:32:DA:H2'	2:O:33:DT:H5''	1.43	0.98
2:O:33:DT:H6	2:O:33:DT:H5'	1.31	0.96
2:M:36:DG:H2''	2:M:37:DT:C5'	1.95	0.95
2:Q:34:DG:H2''	2:Q:35:DA:H5'	1.48	0.94
2:M:30:DT:H2'	2:M:31:DC:C6	2.01	0.94
2:O:32:DA:H2'	2:O:33:DT:C5'	1.98	0.94
2:O:21:DT:H2''	2:O:22:DG:H5''	1.46	0.93
1:D:113:ASN:HD22	1:D:115:SER:H	1.17	0.92
2:K:11:DC:H6	2:K:11:DC:O5'	1.52	0.90
2:O:18:DT:H6	2:O:18:DT:C5'	1.83	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:DT:H5'	3:P:2:DT:C6	2.07	0.89
2:O:17:DC:H2''	2:O:18:DT:H5''	1.52	0.89
2:O:33:DT:H5'	2:O:33:DT:C6	2.08	0.88
2:O:17:DC:H2'	2:O:18:DT:H5''	1.54	0.88
2:O:34:DG:H2''	2:O:35:DA:C5'	2.04	0.88
1:F:113:ASN:HD22	1:F:115:SER:H	1.18	0.87
2:G:11:DC:HO5'	2:G:11:DC:H6	0.94	0.87
1:B:125:THR:HG22	1:B:127:ALA:H	1.39	0.86
2:G:30:DT:H2'	2:G:31:DC:C6	2.11	0.85
2:O:30:DT:H2'	2:O:31:DC:C6	2.13	0.84
1:F:23:HIS:CD2	1:F:121:VAL:HG21	2.14	0.83
2:O:17:DC:H2'	2:O:18:DT:C5'	2.09	0.82
2:Q:22:DG:H2''	2:Q:23:DA:H5'	1.59	0.82
2:Q:24:DC:H2''	2:Q:25:DT:C7	2.08	0.81
1:D:113:ASN:ND2	1:D:115:SER:H	1.76	0.81
2:M:34:DG:H1'	2:M:35:DA:H5''	1.63	0.81
2:O:17:DC:C2'	2:O:18:DT:C5'	2.59	0.81
2:O:23:DA:H2''	2:O:24:DC:H5''	1.62	0.80
1:C:19:GLN:HB3	1:D:119:LEU:HD12	1.63	0.80
1:E:75:THR:HG22	1:E:77:GLN:H	1.47	0.79
2:Q:34:DG:H2''	2:Q:35:DA:C5'	2.13	0.78
2:G:11:DC:H6	2:G:11:DC:O5'	1.66	0.78
3:L:2:DT:H5'	3:L:2:DT:H6	1.47	0.78
1:F:23:HIS:CE1	1:F:71:LEU:HG	2.20	0.77
1:F:113:ASN:ND2	1:F:115:SER:H	1.82	0.76
2:I:36:DG:H2''	2:I:37:DT:H5'	1.67	0.76
2:I:36:DG:H2''	2:I:37:DT:C5'	2.16	0.75
2:Q:24:DC:C2'	2:Q:25:DT:C7	2.65	0.75
1:F:46:ILE:O	1:F:50:ILE:HG13	1.86	0.75
2:K:36:DG:H2''	2:K:37:DT:H5'	1.69	0.75
2:M:12:DG:C2'	2:M:13:DC:H5''	2.13	0.75
1:B:46:ILE:HD12	1:B:95:MET:CE	2.17	0.75
2:O:32:DA:C2'	2:O:33:DT:C5'	2.60	0.73
2:O:18:DT:C6	2:O:18:DT:C5'	2.65	0.72
2:K:34:DG:H2''	2:K:35:DA:H5'	1.71	0.72
1:F:93:ARG:HE	2:Q:27:DC:H5''	1.56	0.71
2:M:30:DT:H2'	2:M:31:DC:H6	1.55	0.71
2:O:36:DG:H2''	2:O:37:DT:C5'	2.21	0.70
2:O:21:DT:H2'	2:O:22:DG:H5''	1.73	0.70
1:E:119:LEU:HD12	1:F:19:GLN:HB3	1.73	0.69
2:O:31:DC:H2'	2:O:32:DA:H8	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:30:DT:H2'	2:Q:31:DC:C6	2.27	0.68
1:D:56:LEU:HD11	1:D:83:PHE:HB2	1.76	0.68
2:O:24:DC:C2'	2:O:25:DT:H72	2.24	0.68
1:C:113:ASN:HD22	1:C:115:SER:H	1.40	0.67
1:A:34:VAL:HG23	1:A:35:LEU:HD13	1.76	0.67
1:A:101:GLN:H	1:A:101:GLN:HE21	1.41	0.67
2:Q:22:DG:H2''	2:Q:23:DA:C5'	2.25	0.66
2:I:15:DC:N3	6:J:1006:GOL:O2	2.23	0.66
2:O:15:DC:N3	6:P:1007:GOL:O2	2.28	0.65
2:G:15:DC:N3	6:G:1038:GOL:O2	2.25	0.65
1:C:34:VAL:O	1:C:39:VAL:HG21	1.96	0.65
1:E:118:ILE:HD12	1:F:18:TYR:HB3	1.79	0.65
1:F:93:ARG:HG2	2:Q:26:DT:H1'	1.79	0.64
2:O:29:DG:H2''	2:O:30:DT:H71	1.79	0.64
2:M:26:DT:H2''	2:M:27:DC:H5'	1.79	0.64
2:K:36:DG:H2''	2:K:37:DT:C5'	2.28	0.64
2:O:11:DC:H2''	2:O:12:DG:O5'	1.98	0.64
1:B:46:ILE:HD12	1:B:95:MET:HE3	1.80	0.63
2:O:31:DC:H2'	2:O:32:DA:C8	2.32	0.63
2:O:34:DG:H1'	2:O:35:DA:H5''	1.79	0.63
1:C:113:ASN:ND2	1:C:115:SER:H	1.97	0.63
1:F:44:LYS:HE3	1:F:63:VAL:HG12	1.79	0.63
2:O:32:DA:H2'	2:O:33:DT:H5'	1.81	0.63
2:Q:30:DT:H2'	2:Q:31:DC:H6	1.62	0.63
2:O:24:DC:H2'	2:O:25:DT:H72	1.81	0.63
2:Q:34:DG:H1'	2:Q:35:DA:H5''	1.79	0.62
3:P:2:DT:H2'	3:P:3:DG:C8	2.34	0.62
2:Q:24:DC:H2'	2:Q:25:DT:H71	1.79	0.62
1:F:48:ARG:HG3	1:F:61:MET:HE1	1.82	0.62
2:M:34:DG:H2''	2:M:35:DA:H5'	1.80	0.62
1:C:36:VAL:O	1:C:39:VAL:HG22	1.99	0.61
2:M:36:DG:C3'	2:M:37:DT:H5''	2.28	0.61
2:M:34:DG:H2''	2:M:35:DA:C5'	2.29	0.61
2:O:28:DA:H5''	2:O:28:DA:N3	2.16	0.61
1:E:99:TYR:HB2	1:E:102:LEU:HD22	1.82	0.60
2:I:30:DT:H2'	2:I:31:DC:C6	2.36	0.60
2:M:19:DC:H2'	2:M:20:DG:H8	1.67	0.60
2:O:36:DG:H2''	2:O:37:DT:H5''	1.83	0.60
2:Q:26:DT:H2''	2:Q:27:DC:H5'	1.83	0.60
1:B:46:ILE:HD12	1:B:95:MET:HE2	1.83	0.60
1:A:134:GLU:C	7:A:2058:HOH:O	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:O	1:D:122:SER:HB3	2.02	0.60
1:E:75:THR:HG22	1:E:77:GLN:N	2.17	0.59
2:O:33:DT:H6	2:O:33:DT:C5'	2.12	0.59
1:F:42:GLY:O	1:F:46:ILE:HG12	2.03	0.59
1:B:126:ARG:O	1:B:130:GLN:HB2	2.03	0.59
2:G:11:DC:H6	2:G:11:DC:C5'	2.16	0.59
1:C:113:ASN:HD22	1:C:113:ASN:C	2.10	0.59
1:E:24:LEU:HD13	1:E:26:TRP:HZ3	1.67	0.59
2:O:32:DA:H2''	2:O:33:DT:H5''	1.79	0.58
1:C:125:THR:OG1	1:C:128:GLN:HG3	2.03	0.57
2:M:11:DC:H6	2:M:11:DC:H5'	1.70	0.57
1:A:56:LEU:HD11	1:A:83:PHE:HB2	1.85	0.57
1:E:77:GLN:NE2	2:Q:32:DA:OP1	2.38	0.57
2:O:34:DG:C2'	2:O:35:DA:C5'	2.79	0.57
3:P:5:DT:C2	6:P:1007:GOL:H32	2.40	0.57
2:Q:30:DT:C2	2:Q:31:DC:C5	2.93	0.56
1:E:75:THR:CG2	1:E:77:GLN:H	2.15	0.56
2:O:21:DT:C2'	2:O:22:DG:C5'	2.77	0.56
2:K:24:DC:H2''	2:K:25:DT:H72	1.87	0.56
3:P:2:DT:H6	3:P:2:DT:C5'	2.05	0.56
2:Q:24:DC:C2	2:Q:25:DT:C4	2.94	0.56
1:A:59:ILE:HD11	1:A:73:SER:HB2	1.86	0.56
1:C:64:MET:HG3	1:C:67:HIS:CE1	2.41	0.56
1:A:125:THR:O	1:A:129:ILE:HG12	2.06	0.56
2:M:34:DG:C1'	2:M:35:DA:H5''	2.35	0.56
2:O:36:DG:H2''	2:O:37:DT:H5'	1.88	0.55
2:Q:19:DC:H2''	2:Q:20:DG:H5'	1.89	0.55
2:O:24:DC:C2'	2:O:25:DT:C7	2.84	0.55
1:D:113:ASN:HD22	1:D:113:ASN:C	2.15	0.55
2:O:17:DC:H2'	2:O:18:DT:H5'	1.86	0.55
2:O:36:DG:C2'	2:O:37:DT:H5''	2.36	0.54
2:Q:12:DG:H1'	2:Q:13:DC:H5''	1.89	0.54
1:F:59:ILE:HD11	1:F:73:SER:HB2	1.90	0.54
2:M:36:DG:C2'	2:M:37:DT:C5'	2.68	0.54
1:F:96:PHE:HD2	2:Q:29:DG:OP1	1.91	0.53
2:Q:34:DG:C2'	2:Q:35:DA:C5'	2.85	0.53
1:F:80:ILE:HB	1:F:81:PRO:HD3	1.90	0.53
1:C:64:MET:HG3	1:C:67:HIS:NE2	2.23	0.53
1:C:113:ASN:HD22	1:C:114:PRO:N	2.06	0.53
1:C:119:LEU:HD12	1:D:19:GLN:HB3	1.91	0.53
2:G:24:DC:H2''	2:G:25:DT:H72	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:19:DC:H2''	2:M:20:DG:H5'	1.90	0.52
2:O:28:DA:N3	2:O:28:DA:H2'	2.23	0.52
1:C:10:MET:CE	1:D:119:LEU:HD11	2.40	0.51
1:C:121:VAL:HG13	1:D:129:ILE:HD12	1.91	0.51
2:O:24:DC:H2''	2:O:25:DT:C7	2.40	0.51
1:D:125:THR:HG22	1:D:127:ALA:H	1.74	0.51
1:B:133:ILE:HG22	7:B:2053:HOH:O	2.09	0.51
1:E:24:LEU:HD13	1:E:26:TRP:CZ3	2.43	0.51
3:L:2:DT:H2'	3:L:3:DG:C8	2.45	0.51
2:Q:27:DC:H6	2:Q:27:DC:O5'	1.93	0.51
3:L:2:DT:H5'	3:L:2:DT:C6	2.38	0.51
1:D:14:ARG:HG2	1:D:14:ARG:HH11	1.76	0.51
1:D:129:ILE:O	1:D:133:ILE:HG12	2.11	0.50
1:A:21:GLU:HA	1:A:72:LEU:O	2.11	0.50
1:E:77:GLN:HE21	2:Q:32:DA:H5''	1.76	0.50
2:Q:24:DC:H2''	2:Q:25:DT:C5	2.46	0.50
2:K:11:DC:O5'	2:K:11:DC:C6	2.41	0.50
1:E:57:GLU:HB3	1:E:73:SER:HB3	1.93	0.50
2:O:12:DG:H2''	2:O:13:DC:O5'	2.12	0.50
1:E:10:MET:SD	1:F:119:LEU:HD21	2.52	0.49
1:F:50:ILE:HD13	1:F:90:ALA:HB3	1.94	0.49
1:B:125:THR:HG22	1:B:127:ALA:N	2.17	0.49
1:A:57:GLU:HB3	1:A:73:SER:HB3	1.93	0.49
2:Q:26:DT:O4	2:Q:30:DT:H1'	2.13	0.49
1:D:113:ASN:HD22	1:D:115:SER:N	1.99	0.49
2:G:30:DT:H2'	2:G:31:DC:H6	1.72	0.49
1:A:9:GLU:HG2	1:A:19:GLN:NE2	2.27	0.48
1:E:56:LEU:HD11	1:E:83:PHE:HB2	1.95	0.48
1:F:75:THR:CG2	1:F:77:GLN:H	2.27	0.48
1:F:113:ASN:HD22	1:F:113:ASN:C	2.21	0.48
1:F:23:HIS:CD2	1:F:121:VAL:CG2	2.93	0.48
2:I:28:DA:H2'	2:I:28:DA:N3	2.29	0.48
3:J:5:DT:C2	6:J:1006:GOL:H32	2.49	0.48
2:Q:31:DC:C2	2:Q:32:DA:C8	3.02	0.48
1:A:133:ILE:CG2	1:B:62:GLU:HG3	2.44	0.48
2:I:27:DC:H2''	7:I:2021:HOH:O	2.14	0.48
1:A:44:LYS:O	1:A:48:ARG:HG3	2.14	0.47
1:E:23:HIS:ND1	1:E:69:HIS:HE1	2.12	0.47
1:A:10:MET:HG2	1:A:17:VAL:HG13	1.95	0.47
1:B:46:ILE:HD13	1:B:94:ARG:HB3	1.95	0.47
1:C:26:TRP:CD1	1:C:88:LYS:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LYS:HA	1:E:106:LEU:O	2.14	0.47
2:M:18:DT:H2'	2:M:19:DC:C6	2.50	0.47
1:B:10:MET:SD	1:B:17:VAL:HG12	2.55	0.47
1:D:137:HIS:ND1	1:D:137:HIS:C	2.72	0.47
2:O:18:DT:H2'	2:O:19:DC:C6	2.49	0.47
2:O:24:DC:C6	2:O:25:DT:H72	2.49	0.47
2:M:26:DT:H2''	2:M:27:DC:C5'	2.44	0.47
2:I:18:DT:H2'	2:I:19:DC:C6	2.50	0.47
1:A:133:ILE:HG22	1:B:62:GLU:HG3	1.97	0.47
2:K:18:DT:H2'	2:K:19:DC:C6	2.50	0.47
1:C:21:GLU:HA	1:C:72:LEU:O	2.13	0.47
1:D:13:GLY:HA3	1:D:16:TYR:CE1	2.50	0.47
2:G:18:DT:H2'	2:G:19:DC:C6	2.50	0.46
2:Q:31:DC:H2'	2:Q:32:DA:H8	1.80	0.46
1:C:19:GLN:HB3	1:D:119:LEU:CD1	2.39	0.46
2:Q:27:DC:H4'	2:Q:28:DA:O4'	2.15	0.46
2:I:20:DG:H2''	2:I:21:DT:H5'	1.97	0.46
2:M:25:DT:H73	2:M:27:DC:N4	2.30	0.46
2:M:34:DG:C2'	2:M:35:DA:H5''	2.45	0.46
2:Q:24:DC:H2'	2:Q:25:DT:C7	2.42	0.46
1:C:48:ARG:HG3	1:C:61:MET:HE1	1.98	0.46
1:E:12:LYS:HD3	2:Q:15:DC:OP1	2.16	0.46
1:E:118:ILE:HD12	1:F:18:TYR:CB	2.46	0.46
1:A:9:GLU:HG2	1:A:19:GLN:HE22	1.81	0.45
1:D:124:ASN:OD1	1:D:128:GLN:NE2	2.49	0.45
2:I:36:DG:C2'	2:I:37:DT:H5''	2.46	0.45
1:C:88:LYS:HE2	2:K:31:DC:OP1	2.16	0.45
2:M:19:DC:H2'	2:M:20:DG:C8	2.49	0.45
2:G:28:DA:N3	2:G:28:DA:H2'	2.32	0.45
1:A:111:LEU:HD13	1:A:112:TRP:CE2	2.52	0.45
2:Q:17:DC:H2'	2:Q:18:DT:C6	2.51	0.45
1:D:23:HIS:ND1	1:D:69:HIS:HE1	2.15	0.45
2:Q:23:DA:H2''	2:Q:24:DC:C6	2.51	0.45
1:E:29:LYS:NZ	2:O:17:DC:OP2	2.49	0.45
1:A:126:ARG:HG2	1:B:123:GLU:OE1	2.17	0.45
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.85	0.45
1:D:113:ASN:HD22	1:D:114:PRO:N	2.15	0.45
2:G:11:DC:C5'	2:G:11:DC:C6	2.99	0.45
1:B:89:GLY:HA3	2:I:26:DT:C4	2.52	0.45
1:D:62:GLU:HB3	1:D:64:MET:HE2	1.98	0.45
2:I:36:DG:H2''	2:I:37:DT:H5''	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:30:DT:H2'	2:O:31:DC:H6	1.76	0.44
1:E:68:VAL:HG12	1:E:70:LEU:HD22	1.99	0.44
1:F:89:GLY:HA3	2:Q:26:DT:C4	2.52	0.44
2:Q:30:DT:C2	2:Q:31:DC:C6	3.05	0.44
1:D:25:ILE:HG23	1:D:68:VAL:O	2.18	0.44
2:M:34:DG:C2'	2:M:35:DA:C5'	2.95	0.44
1:A:84:VAL:HG11	1:A:116:TYR:CD2	2.52	0.44
1:F:63:VAL:HG13	1:F:63:VAL:O	2.18	0.44
1:F:107:TRP:O	3:R:1:DT:O4	2.35	0.44
1:A:23:HIS:ND1	1:A:69:HIS:HE1	2.15	0.44
1:C:78:GLN:HG2	7:C:2022:HOH:O	2.18	0.44
1:B:133:ILE:O	1:B:133:ILE:CG2	2.66	0.43
1:E:120:THR:HG23	1:F:20:LEU:HD23	2.00	0.43
2:O:18:DT:C6	2:O:18:DT:C4'	3.01	0.43
2:O:32:DA:C3'	2:O:33:DT:C5'	2.95	0.43
1:E:91:SER:O	1:E:95:MET:HG2	2.18	0.43
2:O:36:DG:H1'	2:O:37:DT:H5''	1.99	0.43
1:C:44:LYS:O	1:C:48:ARG:HG3	2.18	0.43
2:M:28:DA:H2'	2:M:28:DA:N3	2.33	0.43
1:E:46:ILE:O	1:E:50:ILE:HG13	2.18	0.43
2:I:36:DG:C2'	2:I:37:DT:C5'	2.93	0.43
2:I:36:DG:H1'	2:I:37:DT:H5''	2.00	0.43
7:A:2012:HOH:O	1:B:129:ILE:HD12	2.18	0.43
2:K:11:DC:H2'	2:K:12:DG:C8	2.54	0.43
1:C:26:TRP:CG	1:C:88:LYS:HD2	2.53	0.43
2:G:11:DC:H2'	2:G:12:DG:C8	2.54	0.43
2:K:20:DG:H2'	2:K:21:DT:C6	2.54	0.43
1:D:48:ARG:HG3	1:D:61:MET:HE1	2.01	0.43
3:L:4:DA:H2''	3:L:5:DT:C4	2.53	0.43
1:A:10:MET:HG2	1:A:17:VAL:CG1	2.49	0.42
1:B:80:ILE:O	1:B:84:VAL:HG23	2.19	0.42
1:C:132:TYR:CE1	3:N:5:DT:H73	2.55	0.42
1:F:44:LYS:HE3	1:F:63:VAL:CG1	2.48	0.42
1:F:42:GLY:HA3	1:F:99:TYR:OH	2.19	0.42
1:F:96:PHE:CD2	2:Q:29:DG:OP1	2.72	0.42
2:O:26:DT:H2''	2:O:27:DC:H5'	2.00	0.42
1:A:17:VAL:O	1:B:117:CYS:HA	2.20	0.42
1:D:14:ARG:HG2	1:D:14:ARG:NH1	2.35	0.42
1:B:48:ARG:HG3	1:B:61:MET:HE1	2.00	0.42
2:K:11:DC:H6	2:K:11:DC:HO5'	0.69	0.42
1:A:32:HIS:HE1	3:H:1:DT:O2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ILE:HG13	1:F:95:MET:HE3	2.02	0.42
1:E:75:THR:HB	1:E:78:GLN:OE1	2.20	0.42
3:P:2:DT:C6	3:P:2:DT:C5'	2.92	0.42
2:K:15:DC:N3	6:L:1006:GOL:O2	2.29	0.42
1:F:23:HIS:ND1	1:F:69:HIS:HE1	2.18	0.42
2:G:12:DG:H2''	2:G:13:DC:O5'	2.20	0.42
1:C:57:GLU:HB3	1:C:73:SER:HB3	2.00	0.42
2:I:24:DC:H2''	2:I:25:DT:H72	2.01	0.42
1:C:23:HIS:CE1	1:D:133:ILE:HD11	2.54	0.41
1:F:25:ILE:HA	1:F:68:VAL:O	2.20	0.41
2:M:17:DC:H2'	2:M:18:DT:C6	2.55	0.41
1:C:13:GLY:HA3	1:C:16:TYR:CE2	2.56	0.41
1:D:14:ARG:HG2	1:D:14:ARG:O	2.19	0.41
3:L:5:DT:C2	6:L:1006:GOL:H32	2.56	0.41
1:A:101:GLN:O	1:A:104:GLU:HG2	2.19	0.41
1:B:129:ILE:O	1:B:133:ILE:HB	2.20	0.41
1:D:77:GLN:N	1:D:77:GLN:CD	2.78	0.41
2:G:13:DC:H5''	2:G:37:DT:C4	2.56	0.41
1:C:56:LEU:HD11	1:C:83:PHE:HB2	2.03	0.41
1:A:125:THR:HG22	1:A:126:ARG:N	2.35	0.41
2:K:34:DG:H1'	2:K:35:DA:H5''	2.01	0.41
2:O:23:DA:H2''	2:O:24:DC:C5'	2.41	0.41
2:O:33:DT:C5'	2:O:33:DT:C6	2.92	0.41
2:Q:34:DG:C1'	2:Q:35:DA:H5''	2.50	0.41
1:E:118:ILE:CD1	1:F:18:TYR:HB3	2.48	0.41
1:F:75:THR:HB	1:F:78:GLN:HG3	2.03	0.41
2:O:20:DG:H2''	2:O:21:DT:H5'	2.03	0.41
1:B:11:LYS:HE3	1:B:19:GLN:HE21	1.85	0.40
1:D:20:LEU:O	1:D:73:SER:HA	2.21	0.40
1:E:123:GLU:HA	1:E:123:GLU:OE2	2.21	0.40
1:F:75:THR:HG22	1:F:77:GLN:H	1.87	0.40
2:M:24:DC:H2''	2:M:25:DT:OP2	2.22	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	124/140 (89%)	119 (96%)	4 (3%)	1 (1%)	16	20
1	B	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
1	C	126/140 (90%)	125 (99%)	1 (1%)	0	100	100
1	D	127/140 (91%)	123 (97%)	3 (2%)	1 (1%)	16	20
1	E	124/140 (89%)	123 (99%)	1 (1%)	0	100	100
1	F	124/140 (89%)	121 (98%)	3 (2%)	0	100	100
All	All	752/840 (90%)	736 (98%)	14 (2%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	D	124	ASN

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	108/122 (88%)	101 (94%)	7 (6%)	15	22
1	B	111/122 (91%)	105 (95%)	6 (5%)	20	29
1	C	110/122 (90%)	105 (96%)	5 (4%)	24	37
1	D	111/122 (91%)	103 (93%)	8 (7%)	13	18
1	E	108/122 (88%)	99 (92%)	9 (8%)	10	14
1	F	108/122 (88%)	101 (94%)	7 (6%)	15	22
All	All	656/732 (90%)	614 (94%)	42 (6%)	16	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	11	LYS
1	A	35	LEU
1	A	60	THR
1	A	101	GLN
1	A	111	LEU
1	A	134	GLU
1	B	72	LEU
1	B	111	LEU
1	B	118	ILE
1	B	120	THR
1	B	126	ARG
1	B	129	ILE
1	C	10	MET
1	C	35	LEU
1	C	62	GLU
1	C	64	MET
1	C	113	ASN
1	D	10	MET
1	D	14	ARG
1	D	43	LEU
1	D	113	ASN
1	D	118	ILE
1	D	123	GLU
1	D	126	ARG
1	D	137	HIS
1	E	24	LEU
1	E	29	LYS
1	E	35	LEU
1	E	75	THR
1	E	102	LEU
1	E	111	LEU
1	E	118	ILE
1	E	121	VAL
1	E	122	SER
1	F	68	VAL
1	F	71	LEU
1	F	75	THR
1	F	88	LYS
1	F	113	ASN
1	F	118	ILE
1	F	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	32	HIS
1	A	69	HIS
1	A	101	GLN
1	A	130	GLN
1	C	113	ASN
1	D	69	HIS
1	D	113	ASN
1	E	19	GLN
1	E	69	HIS
1	E	77	GLN
1	F	23	HIS
1	F	69	HIS
1	F	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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
6	GOL	G	1038	-	5,5,5	0.70	0	5,5,5	0.38	0
6	GOL	L	1006	-	5,5,5	0.47	0	5,5,5	0.29	0
4	ACT	B	1135	-	3,3,3	0.73	0	3,3,3	0.80	0
6	GOL	P	1007	-	5,5,5	0.74	0	5,5,5	0.32	0
6	GOL	J	1006	-	5,5,5	0.66	0	5,5,5	0.54	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
6	GOL	G	1038	-	-	0/4/4/4	-
6	GOL	P	1007	-	-	0/4/4/4	-
6	GOL	J	1006	-	-	0/4/4/4	-
6	GOL	L	1006	-	-	0/4/4/4	-

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1038	GOL	1	0
6	L	1006	GOL	2	0
6	P	1007	GOL	2	0
6	J	1006	GOL	2	0

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, 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	126/140 (90%)	-0.18	4 (3%)	50	52	17, 30, 65, 98	0
1	B	129/140 (92%)	-0.10	7 (5%)	31	33	19, 32, 63, 90	0
1	C	128/140 (91%)	-0.16	5 (3%)	43	45	19, 30, 66, 97	0
1	D	129/140 (92%)	0.02	12 (9%)	14	16	19, 33, 85, 106	0
1	E	126/140 (90%)	0.28	10 (7%)	18	20	22, 39, 81, 107	0
1	F	126/140 (90%)	0.61	10 (7%)	18	20	23, 44, 71, 79	0
2	G	27/27 (100%)	-0.58	0	100	100	24, 34, 49, 59	0
2	I	27/27 (100%)	-0.59	1 (3%)	45	48	22, 35, 43, 52	0
2	K	27/27 (100%)	-0.87	0	100	100	18, 28, 38, 49	0
2	M	27/27 (100%)	-0.48	0	100	100	26, 36, 52, 62	0
2	O	27/27 (100%)	0.72	3 (11%)	10	11	31, 53, 68, 77	0
2	Q	27/27 (100%)	0.53	2 (7%)	20	22	28, 46, 75, 79	0
3	H	5/5 (100%)	-0.93	0	100	100	25, 30, 35, 37	0
3	J	5/5 (100%)	-0.89	0	100	100	26, 28, 29, 29	0
3	L	5/5 (100%)	-0.57	0	100	100	29, 29, 31, 35	0
3	N	5/5 (100%)	-0.85	0	100	100	30, 31, 33, 36	0
3	P	5/5 (100%)	-0.36	0	100	100	33, 35, 43, 46	0
3	R	5/5 (100%)	-0.80	0	100	100	30, 32, 34, 43	0
All	All	956/1032 (92%)	0.00	54 (5%)	30	32	17, 35, 72, 107	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	HIS	4.8
1	B	130	GLN	4.2
1	D	131	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	133	ILE	4.0
1	D	132	TYR	3.7
1	D	127	ALA	3.7
2	O	11	DC	3.6
1	D	129	ILE	3.5
1	C	132	TYR	3.3
1	D	133	ILE	3.3
1	F	97	VAL	3.3
1	E	132	TYR	3.2
1	C	7	PRO	3.2
1	D	130	GLN	3.0
1	F	96	PHE	3.0
1	E	134	GLU	3.0
1	B	133	ILE	2.9
1	F	100	PRO	2.9
1	B	129	ILE	2.9
1	E	131	LYS	2.7
1	C	134	GLU	2.7
1	E	123	GLU	2.6
1	D	135	SER	2.6
2	O	12	DG	2.5
1	F	39	VAL	2.5
1	A	134	GLU	2.5
1	E	126	ARG	2.5
1	C	133	ILE	2.4
2	I	12	DG	2.4
1	D	125	THR	2.4
1	F	98	ALA	2.4
1	F	108	GLY	2.4
1	A	129	ILE	2.4
1	F	93	ARG	2.4
2	Q	22	DG	2.4
1	E	127	ALA	2.4
1	C	131	LYS	2.3
2	O	21	DT	2.3
1	B	126	ARG	2.2
1	E	9	GLU	2.2
1	E	129	ILE	2.2
1	B	6	LEU	2.2
1	D	123	GLU	2.2
1	A	132	TYR	2.1
1	B	7	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	99	TYR	2.1
1	D	126	ARG	2.1
1	B	134	GLU	2.1
1	E	125	THR	2.0
1	F	9	GLU	2.0
1	D	124	ASN	2.0
1	A	133	ILE	2.0
2	Q	26	DT	2.0
1	F	102	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	B	1135	4/4	0.66	0.17	62,63,63,63	0
6	GOL	J	1006	6/6	0.83	0.20	44,45,46,48	0
6	GOL	L	1006	6/6	0.84	0.21	44,48,48,50	0
6	GOL	G	1038	6/6	0.85	0.17	46,46,47,48	0
6	GOL	P	1007	6/6	0.89	0.15	40,41,43,43	0
5	MG	F	1135	1/1	0.96	0.05	39,39,39,39	0
5	MG	E	1135	1/1	0.97	0.04	35,35,35,35	0
5	MG	K	1038	1/1	0.97	0.04	21,21,21,21	0
5	MG	I	1038	1/1	0.98	0.03	26,26,26,26	0
5	MG	G	1039	1/1	0.98	0.06	23,23,23,23	0
5	MG	K	1039	1/1	0.98	0.04	34,34,34,34	0
5	MG	O	1112	1/1	0.98	0.05	52,52,52,52	0
5	MG	G	1114	1/1	0.99	0.03	36,36,36,36	0
5	MG	Q	1111	1/1	0.99	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	M	1038	1/1	0.99	0.05	24,24,24,24	0
5	MG	I	1116	1/1	1.00	0.01	34,34,34,34	0
5	MG	M	1121	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.