



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1Z19
Title : Crystal structure of a lambda integrase(75-356) dimer bound to a COC' core site
Authors : Biswas, T.; Aihara, H.; Radman-Livaja, M.; Filman, D.; Landy, A.; Ellenberger, T.
Deposited on : 2005-03-03
Resolution : 2.80 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

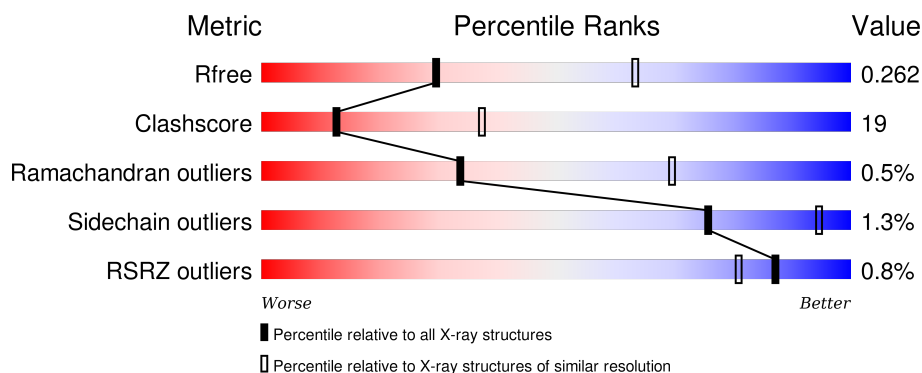
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	C	16	<div> <div>6%</div> <div>56%</div> <div>19%</div> <div>19%</div> </div>
2	D	20	<div> <div>10%</div> <div>5%</div> <div>95%</div> </div>
3	E	33	<div> <div>6%</div> <div>15%</div> <div>79%</div> <div>6%</div> </div>
4	A	283	<div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
4	B	283	<div> <div>76%</div> <div>24%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5677 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 5'-D(*CP*TP*CP*GP*TP*TP*CP*AP*GP*CP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	0	0	1
			243	117	36	78	12			

- Molecule 2 is a DNA chain called 5'-D(P*TP*TP*TP*AP*TP*AP*CP*TP*AP*AP*GP*T*TP*GP*GP*CP*AP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	P	0	0	0
			394	188	64	122	20			

- Molecule 3 is a DNA chain called 33-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	33	Total	C	N	O	P	0	0	0
			679	325	134	188	32			

- Molecule 4 is a protein called Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	273	Total	C	N	O	S	Se	0	0	0
			2111	1333	374	393	3	8			
4	B	283	Total	C	N	O	P	S	Se	0	0
			2219	1391	397	419	1	3	8		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MSE	VAL	SEE REMARK 999	UNP P03700
A	101	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	127	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	174	LYS	GLU	ENGINEERED	UNP P03700

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Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	219	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	255	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	290	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	338	MSE	MET	MODIFIED RESIDUE	UNP P03700
A	342	PTR	TYR	MODIFIED RESIDUE	UNP P03700
B	74	MSE	VAL	SEE REMARK 999	UNP P03700
B	101	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	127	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	174	LYS	GLU	ENGINEERED	UNP P03700
B	203	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	219	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	255	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	290	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	338	MSE	MET	MODIFIED RESIDUE	UNP P03700
B	342	PTR	TYR	MODIFIED RESIDUE	UNP P03700

- Molecule 5 is water.

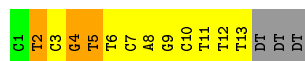
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	15	Total O 15 15	0	0
5	C	4	Total O 4 4	0	0

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.

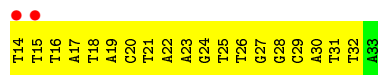
- Molecule 1: 5'-D(*CP*TP*CP*GP*TP*TP*CP*AP*GP*CP*TP*TP*TP*TP*TP*T)-3'

Chain C: 



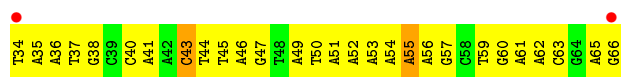
- Molecule 2: 5'-D(P*TP*TP*TP*AP*TP*AP*CP*TP*AP*AP*GP*TP*TP*GP*GP*CP*AP*TP*TP*A)-3'

Chain D: 



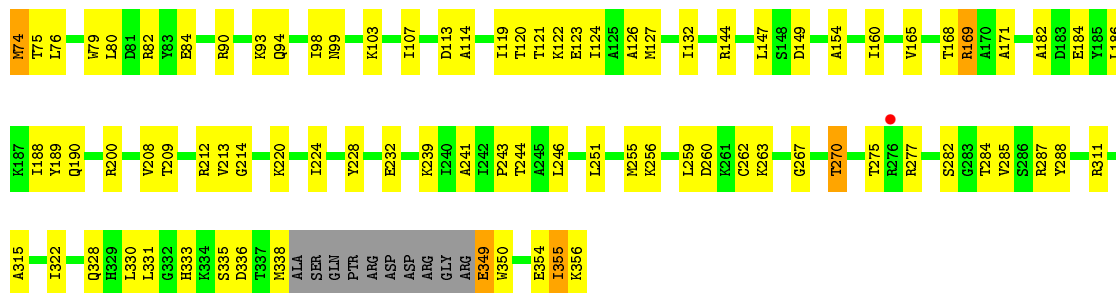
- Molecule 3: 33-MER

Chain E: 



- Molecule 4: Integrase

Chain A: 



- Molecule 4: Integrase

Chain B: 

L201	L205	T209	G210	G211	L216	W221	G227	T244	L248	M255	G262	L266	G267	G268	T275	R287	M290	S296	G297	L298	E309	L313	R316	L317	Y318	E319	D324	S335	R343	K352	L353	E354	L355	K356							
M74	T75	L76	H77	D81	K93	L97	M101	R108	L111	P112	D113	A114	P115	L116	I119	T120	E123	I124	M127	L128	G129	G130	Y131	I132	A138	R144	S145	G158	H159	L160	T161	V165	T168	R169	A170	R179	L180	T181	E184	K187	L189

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.30 Å 121.48 Å 65.39 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 98.7 (49.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.81 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.262 0.214 , 0.262	Depositor DCC
R_{free} test set	2226 reflections (11.36%)	DCC
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22095 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PTR

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	C	0.54	0/269	0.92	1/414 (0.2%)
2	D	0.53	0/439	0.87	0/675
3	E	0.51	0/765	0.85	1/1179 (0.1%)
4	A	0.42	0/2138	0.61	0/2868
4	B	0.42	0/2231	0.61	0/2988
All	All	0.45	0/5842	0.69	2/8124 (0.0%)

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	C	0	3
3	E	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	DT	N1-C1'-C2'	5.27	122.61	112.60
3	E	59	DT	N1-C1'-C2'	5.21	122.51	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	C	4	DG	Sidechain
1	C	5	DT	Sidechain
3	E	43	DC	Sidechain
3	E	55	DA	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	C	243	0	138	19	0
2	D	394	0	218	28	0
3	E	679	0	372	48	0
4	A	2111	0	2137	67	0
4	B	2219	0	2247	60	0
5	A	12	0	0	0	0
5	B	15	0	0	1	0
5	C	4	0	0	0	0
All	All	5677	0	5112	208	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 19.

All (208) 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)
4:A:120:THR:HG22	4:A:122:LYS:H	1.20	1.06
4:A:165:VAL:O	4:A:168:THR:HG22	1.62	0.99
4:B:244:THR:HA	4:B:255:MSE:HE2	1.49	0.94
4:A:120:THR:HG22	4:A:122:LYS:N	1.83	0.93
4:B:120:THR:HG22	4:B:123:GLU:OE1	1.70	0.89
2:D:20:DC:H2''	2:D:21:DT:H5'	1.55	0.86
4:A:144:ARG:HE	4:A:168:THR:HG23	1.40	0.85
3:E:40:DC:H2''	3:E:41:DA:H5'	1.55	0.85
4:B:120:THR:HG23	4:B:123:GLU:H	1.42	0.85
4:B:160:ILE:HG22	4:B:161:THR:H	1.43	0.82
4:B:187:LYS:HD2	4:B:298:LEU:HD21	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:DT:H5'	4:B:335:SER:HB3	1.60	0.80
2:D:27:DG:N7	4:A:287:ARG:NH2	2.33	0.76
3:E:60:DG:H2''	3:E:61:DA:H5'	1.69	0.74
4:A:243:PRO:HG2	4:A:246:LEU:CD1	2.17	0.74
4:A:74:MSE:SE	4:A:74:MSE:N	2.71	0.74
3:E:60:DG:H2''	3:E:61:DA:C5'	2.18	0.73
4:A:79:TRP:CZ3	4:A:82:ARG:HG2	2.25	0.72
3:E:65:DA:H1'	3:E:66:DG:H5''	1.71	0.71
3:E:51:DA:H2''	3:E:52:DA:H5'	1.74	0.70
4:A:186:LEU:O	4:A:190:GLN:HG3	1.93	0.68
2:D:20:DC:H2''	2:D:21:DT:C5'	2.22	0.68
4:A:315:ALA:HB2	4:A:331:LEU:HD11	1.76	0.68
4:B:124:ILE:HD13	4:B:165:VAL:HG22	1.76	0.68
1:C:3:DC:H2''	1:C:4:DG:C5'	2.24	0.68
1:C:3:DC:H2''	1:C:4:DG:H5'	1.75	0.67
2:D:14:DT:H5''	2:D:15:DT:H71	1.76	0.67
4:B:77:HIS:HB2	4:B:113:ASP:OD1	1.94	0.67
2:D:25:DT:H2''	2:D:26:DT:H5'	1.75	0.66
3:E:56:DA:H2'	3:E:57:DG:C8	2.31	0.66
2:D:15:DT:H1'	2:D:16:DT:OP1	1.96	0.66
2:D:23:DA:H2'	2:D:24:DG:C8	2.31	0.66
4:A:322:ILE:HD13	4:B:355:ILE:HG23	1.78	0.66
3:E:40:DC:C2'	3:E:41:DA:H5'	2.25	0.65
4:B:227:GLY:O	4:B:244:THR:HG23	1.98	0.64
4:A:169:ARG:HD2	4:A:169:ARG:O	1.97	0.64
4:B:97:LEU:HD23	4:B:101:MSE:HG2	1.80	0.63
1:C:10:DC:H2'	1:C:11:DT:H72	1.81	0.62
4:B:76:LEU:HD22	4:B:119:ILE:HD13	1.81	0.62
4:B:287:ARG:O	4:B:290:MSE:HE3	2.00	0.62
3:E:43:DC:H2'	3:E:44:DT:H72	1.81	0.62
4:A:241:ALA:HB3	4:B:352:LYS:HA	1.80	0.62
2:D:23:DA:C2'	2:D:24:DG:C8	2.83	0.62
3:E:36:DA:H2''	3:E:37:DT:H5''	1.81	0.61
3:E:52:DA:H2''	3:E:53:DA:H5'	1.83	0.61
4:A:90:ARG:NH2	4:B:169:ARG:HH12	1.98	0.61
4:A:169:ARG:HD2	4:A:169:ARG:C	2.22	0.61
3:E:56:DA:C2'	3:E:57:DG:C8	2.84	0.60
4:B:81:ASP:OD1	4:B:108:ARG:NH2	2.34	0.60
4:A:144:ARG:HE	4:A:168:THR:CG2	2.14	0.60
3:E:46:DA:H2''	4:A:338:MSE:HE1	1.82	0.60
4:B:244:THR:HA	4:B:255:MSE:CE	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:34:DT:C3'	3:E:35:DA:H5''	2.31	0.60
4:B:181:THR:OG1	4:B:184:GLU:HG3	2.01	0.60
3:E:36:DA:H2''	3:E:37:DT:C5'	2.32	0.60
2:D:29:DC:H2''	2:D:30:DA:OP2	2.02	0.59
4:A:244:THR:O	4:A:256:LYS:HG3	2.03	0.59
3:E:56:DA:C2'	3:E:57:DG:H8	2.15	0.59
2:D:31:DT:H1'	2:D:32:DT:H5'	1.84	0.58
4:A:149:ASP:OD1	4:B:169:ARG:NH2	2.37	0.58
3:E:52:DA:H2''	3:E:53:DA:C5'	2.34	0.57
4:B:76:LEU:HB2	4:B:119:ILE:HD11	1.86	0.57
4:A:208:VAL:HG13	4:A:209:THR:HG23	1.87	0.56
3:E:34:DT:H2''	3:E:35:DA:H5''	1.86	0.56
4:A:182:ALA:HB1	4:A:251:LEU:HD21	1.86	0.56
3:E:36:DA:H1'	3:E:37:DT:H5''	1.86	0.56
1:C:5:DT:C2'	1:C:6:DT:H72	2.36	0.56
4:B:144:ARG:HE	4:B:168:THR:HG22	1.71	0.56
3:E:36:DA:C2'	3:E:37:DT:H5''	2.35	0.56
4:A:107:ILE:HD13	4:A:147:LEU:HD13	1.88	0.56
2:D:14:DT:H5'	4:B:335:SER:CB	2.32	0.55
1:C:11:DT:H1'	1:C:12:DT:H5''	1.88	0.55
4:A:232:GLU:OE2	4:A:239:LYS:HE2	2.06	0.55
3:E:46:DA:H4'	3:E:47:DG:OP1	2.06	0.55
3:E:34:DT:C2'	3:E:35:DA:H5''	2.37	0.55
2:D:20:DC:H1'	2:D:21:DT:H5''	1.89	0.55
4:B:75:THR:CG2	4:B:113:ASP:OD1	2.54	0.55
4:B:319:GLU:OE2	4:B:324:ASP:HA	2.06	0.55
3:E:49:DA:H1'	3:E:50:DT:H5''	1.89	0.55
4:B:168:THR:CG2	4:B:169:ARG:N	2.70	0.55
1:C:7:DC:H1'	1:C:8:DA:H5''	1.89	0.55
1:C:5:DT:C6	1:C:6:DT:H72	2.41	0.55
4:B:184:GLU:O	4:B:188:ILE:HG13	2.06	0.54
4:B:205:LEU:O	4:B:209:THR:HG23	2.07	0.54
4:A:224:ILE:HA	4:A:228:TYR:O	2.07	0.54
4:A:213:VAL:HG13	4:A:282:SER:HB2	1.90	0.54
2:D:15:DT:C1'	2:D:16:DT:OP1	2.56	0.54
1:C:10:DC:C6	1:C:11:DT:H72	2.42	0.54
1:C:7:DC:H2''	1:C:8:DA:H5'	1.88	0.54
1:C:10:DC:H2'	1:C:11:DT:C7	2.38	0.54
3:E:56:DA:H2'	3:E:57:DG:H8	1.70	0.53
4:B:127:MSE:HE3	4:B:128:LEU:HD23	1.90	0.53
1:C:4:DG:OP1	4:B:275:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:120:THR:HG22	4:A:121:THR:N	2.24	0.52
4:B:97:LEU:HD21	4:B:101:MSE:HE3	1.90	0.52
4:B:187:LYS:CD	4:B:298:LEU:HD21	2.37	0.52
2:D:14:DT:H2'	2:D:15:DT:C7	2.39	0.52
3:E:53:DA:H1'	3:E:54:DA:H5'	1.91	0.52
4:B:169:ARG:O	4:B:169:ARG:HG3	2.09	0.52
1:C:3:DC:H1'	1:C:4:DG:H5''	1.92	0.52
4:A:275:THR:C	4:A:277:ARG:H	2.13	0.52
4:A:335:SER:OG	4:A:336:ASP:N	2.43	0.51
3:E:38:DG:H5'	3:E:38:DG:H8	1.74	0.51
4:A:330:LEU:HA	4:B:353:ILE:HD13	1.91	0.51
3:E:43:DC:H2''	3:E:44:DT:C6	2.46	0.51
3:E:47:DG:H4'	4:A:212:ARG:NH2	2.25	0.51
4:B:158:GLY:HA2	5:B:19:HOH:O	2.10	0.51
4:B:160:ILE:HG22	4:B:161:THR:N	2.20	0.50
4:A:75:THR:HG22	4:A:113:ASP:OD1	2.12	0.50
2:D:27:DG:H2''	2:D:28:DG:H5'	1.94	0.50
3:E:60:DG:H1'	3:E:61:DA:H5''	1.93	0.50
3:E:37:DT:H71	4:A:288:TYR:OH	2.12	0.49
4:A:355:ILE:HG22	4:A:355:ILE:O	2.12	0.49
2:D:14:DT:H2'	2:D:15:DT:H71	1.93	0.49
4:B:127:MSE:HE3	4:B:128:LEU:CD2	2.42	0.49
4:A:259:LEU:O	4:A:262:CYS:HB2	2.13	0.49
4:B:180:LEU:O	4:B:313:LEU:HD13	2.13	0.49
3:E:52:DA:H1'	3:E:53:DA:H5''	1.94	0.49
4:A:120:THR:CG2	4:A:121:THR:N	2.75	0.49
1:C:2:DT:H2''	1:C:3:DC:C6	2.48	0.49
3:E:60:DG:C2'	3:E:61:DA:H5''	2.42	0.48
4:A:244:THR:HG22	4:A:255:MSE:HE2	1.95	0.48
4:A:94:GLN:O	4:A:98:ILE:HG13	2.13	0.48
4:B:296:SER:OG	4:B:298:LEU:HG	2.13	0.48
3:E:60:DG:H2''	3:E:61:DA:H5''	1.94	0.48
4:B:168:THR:HG22	4:B:169:ARG:N	2.27	0.48
4:A:76:LEU:HD22	4:A:119:ILE:CD1	2.43	0.48
2:D:15:DT:H2''	2:D:16:DT:C5	2.48	0.48
4:A:311:ARG:HH21	4:A:333:HIS:HE1	1.62	0.48
2:D:17:DA:H2''	2:D:18:DT:OP2	2.13	0.47
2:D:23:DA:H2''	2:D:24:DG:C8	2.48	0.47
4:B:201:LEU:HD12	4:B:266:LEU:HD11	1.95	0.47
4:A:120:THR:CG2	4:A:122:LYS:H	2.08	0.47
4:A:76:LEU:HD22	4:A:119:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:132:ILE:HD11	4:A:171:ALA:HB2	1.96	0.47
2:D:20:DC:C2'	2:D:21:DT:C5'	2.93	0.47
4:B:221:TRP:CD1	4:B:268:GLY:O	2.68	0.46
2:D:17:DA:H1'	2:D:18:DT:H5'	1.96	0.46
4:A:260:ASP:O	4:A:263:LYS:HG2	2.15	0.46
4:B:132:ILE:HD11	4:B:171:ALA:HB2	1.97	0.46
2:D:19:DA:H1'	2:D:20:DC:H5''	1.97	0.46
4:B:165:VAL:O	4:B:168:THR:HB	2.16	0.46
4:B:209:THR:O	4:B:211:GLN:NE2	2.42	0.46
3:E:56:DA:H2''	3:E:57:DG:H8	1.81	0.45
2:D:23:DA:C2'	2:D:24:DG:H8	2.28	0.45
2:D:16:DT:H2''	2:D:17:DA:OP2	2.16	0.45
4:B:316:ARG:O	4:B:319:GLU:HB3	2.16	0.45
4:A:123:GLU:O	4:A:126:ALA:HB3	2.15	0.45
3:E:40:DC:H1'	3:E:41:DA:C5'	2.47	0.45
4:B:144:ARG:HH11	4:B:144:ARG:HG2	1.82	0.45
3:E:56:DA:H2''	3:E:57:DG:C8	2.50	0.45
4:B:74:MSE:O	4:B:115:PRO:HA	2.17	0.45
4:A:220:LYS:HA	4:A:270:THR:HA	1.98	0.45
3:E:49:DA:H1'	3:E:50:DT:C5'	2.47	0.44
4:A:80:LEU:O	4:A:84:GLU:HG3	2.18	0.44
4:B:111:LEU:HA	4:B:112:PRO:HD3	1.76	0.44
4:B:128:LEU:O	4:B:132:ILE:HG13	2.17	0.44
4:B:262:CYS:O	4:B:266:LEU:HB2	2.17	0.44
4:B:216:LEU:HD12	4:B:216:LEU:HA	1.77	0.44
4:A:189:TYR:CE1	4:A:200:ARG:HD3	2.52	0.44
4:A:144:ARG:NE	4:A:168:THR:HG23	2.20	0.43
1:C:5:DT:H2''	1:C:6:DT:C7	2.48	0.43
3:E:44:DT:H1'	3:E:45:DT:H5''	1.99	0.43
4:A:184:GLU:O	4:A:188:ILE:HG13	2.19	0.43
4:A:311:ARG:NH2	4:A:333:HIS:HE1	2.16	0.43
4:B:324:ASP:N	4:B:324:ASP:OD2	2.51	0.43
3:E:61:DA:H2''	3:E:62:DA:C8	2.54	0.43
3:E:56:DA:H8	3:E:56:DA:C5'	2.32	0.43
4:A:99:ASN:O	4:A:103:LYS:HG2	2.18	0.43
4:B:97:LEU:CD2	4:B:101:MSE:HE3	2.49	0.42
3:E:43:DC:H2'	3:E:44:DT:C7	2.47	0.42
4:B:127:MSE:O	4:B:130:GLY:N	2.52	0.42
4:A:124:ILE:HD13	4:A:165:VAL:HG22	2.01	0.42
4:A:75:THR:HG23	4:A:114:ALA:C	2.39	0.42
4:A:74:MSE:HB2	4:A:75:THR:H	1.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:DA:H3'	4:A:93:LYS:HD3	2.00	0.42
3:E:38:DG:C8	3:E:38:DG:H5'	2.54	0.42
4:A:76:LEU:HB2	4:A:119:ILE:HD11	2.02	0.42
3:E:40:DC:H1'	3:E:41:DA:H5'	2.00	0.42
4:A:311:ARG:NH2	4:A:333:HIS:CE1	2.87	0.42
4:A:349:GLU:HB2	4:A:350:TRP:H	1.59	0.42
2:D:22:DA:H1'	2:D:23:DA:H5''	2.02	0.42
4:A:127:MSE:HE2	4:A:127:MSE:HB3	1.93	0.42
1:C:11:DT:OP2	4:B:138:ALA:HB3	2.20	0.41
4:B:319:GLU:OE1	4:B:343:ARG:HD3	2.20	0.41
4:A:243:PRO:HG2	4:A:246:LEU:HD11	2.00	0.41
4:B:116:LEU:HA	4:B:119:ILE:HD12	2.02	0.41
4:B:248:ILE:HD11	4:B:318:TYR:CZ	2.55	0.41
3:E:60:DG:C2'	3:E:61:DA:C5'	2.92	0.41
3:E:49:DA:H2''	3:E:50:DT:OP2	2.21	0.41
4:B:179:ARG:HD3	4:B:309:GLU:OE1	2.20	0.41
3:E:62:DA:H1'	3:E:63:DC:H5'	2.01	0.41
1:C:9:DG:H1'	1:C:10:DC:H5''	2.02	0.41
1:C:5:DT:H2'	1:C:6:DT:H72	2.02	0.41
4:A:147:LEU:HA	4:A:147:LEU:HD12	1.90	0.41
4:A:213:VAL:HG13	4:A:214:GLY:N	2.36	0.41
3:E:43:DC:H2''	3:E:44:DT:H6	1.86	0.41
1:C:5:DT:H2''	1:C:6:DT:OP2	2.21	0.41
4:A:328:GLN:OE1	4:A:335:SER:O	2.39	0.41
1:C:3:DC:H2''	1:C:4:DG:H5''	2.01	0.40
3:E:55:DA:H1'	3:E:56:DA:H5''	2.02	0.40
3:E:36:DA:C1'	3:E:37:DT:H5''	2.51	0.40
2:D:30:DA:H2''	2:D:31:DT:OP2	2.22	0.40
4:B:317:LEU:HD23	4:B:317:LEU:HA	1.86	0.40
4:A:284:THR:O	4:A:285:VAL:C	2.60	0.40
4:A:154:ALA:HB3	4:A:160:ILE:HD11	2.03	0.40
4:A:213:VAL:CG1	4:A:214:GLY:N	2.85	0.40
4:A:354:GLU:C	4:A:356:LYS:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	269/283 (95%)	253 (94%)	14 (5%)	2 (1%)	26	62
4	B	280/283 (99%)	263 (94%)	16 (6%)	1 (0%)	39	74
All	All	549/566 (97%)	516 (94%)	30 (6%)	3 (0%)	34	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	267	GLY
4	B	267	GLY
4	A	355	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	219/228 (96%)	215 (98%)	4 (2%)	66	91
4	B	232/228 (102%)	230 (99%)	2 (1%)	84	96
All	All	451/456 (99%)	445 (99%)	6 (1%)	76	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	74	MSE
4	A	169	ARG
4	A	270	THR

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Mol	Chain	Res	Type
4	A	349	GLU
4	B	93	LYS
4	B	145	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	159	HIS
4	A	329	HIS
4	A	333	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PTR	B	342	1,4	11,15,17	0.62	0	13,19,24	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PTR	B	342	1,4	-	0/6/10/13	0/1/1/1

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	C	13/16 (81%)	-0.05	0 100 100	36, 58, 72, 95	0
2	D	20/20 (100%)	0.17	2 (10%) 9 4	34, 64, 146, 150	0
3	E	33/33 (100%)	-0.02	2 (6%) 25 15	34, 51, 84, 94	2 (6%)
4	A	265/283 (93%)	-0.07	1 (0%) 93 90	31, 54, 73, 108	0
4	B	274/283 (96%)	-0.17	0 100 100	33, 49, 71, 89	0
All	All	605/635 (95%)	-0.10	5 (0%) 87 81	31, 52, 75, 150	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	34	DT	3.4
3	E	66	DG	3.1
2	D	14	DT	2.7
2	D	15	DT	2.6
4	A	276	ARG	2.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PTR	B	342	15/17	0.98	0.19	-	39,43,48,50	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.