



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:02 am BST

PDB ID : 5TGX
Title : Restriction/modification system-Type II R-SwaI complexed with partially cleaved DNA
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2016-09-28
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

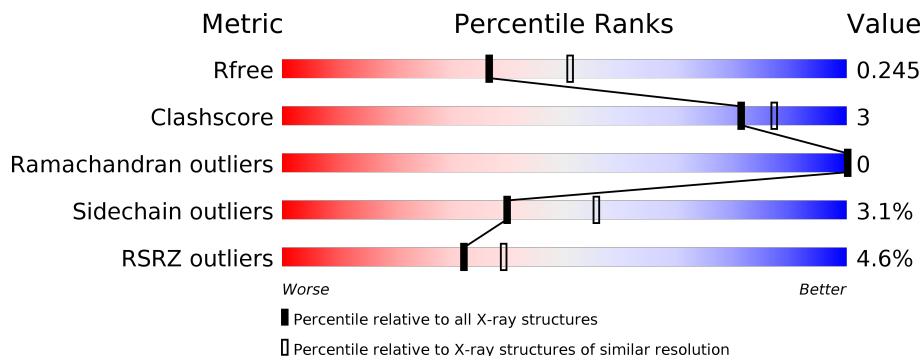
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



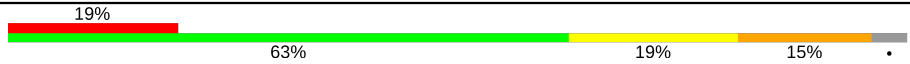

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	226	
1	B	226	
1	C	226	
1	D	226	
2	H	27	
2	J	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	27	
3	K	27	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10136 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 R-Swal protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	225	Total 1894	C 1217	N 314	O 358	S 1	Se 4	0	1	0
1	B	225	Total 1891	C 1216	N 314	O 356	S 1	Se 4	0	1	0
1	C	225	Total 1904	C 1223	N 315	O 361	S 1	Se 4	0	3	0
1	D	225	Total 1894	C 1217	N 315	O 357	S 1	Se 4	0	1	0

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	H	26	Total 582	C 274	N 113	O 167	P 28	0	2	0
2	J	27	Total 601	C 284	N 118	O 171	P 28	0	2	0

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	I	26	Total 563	C 269	N 100	O 167	P 27	0	2	0
3	K	26	Total 563	C 269	N 100	O 167	P 27	1	2	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

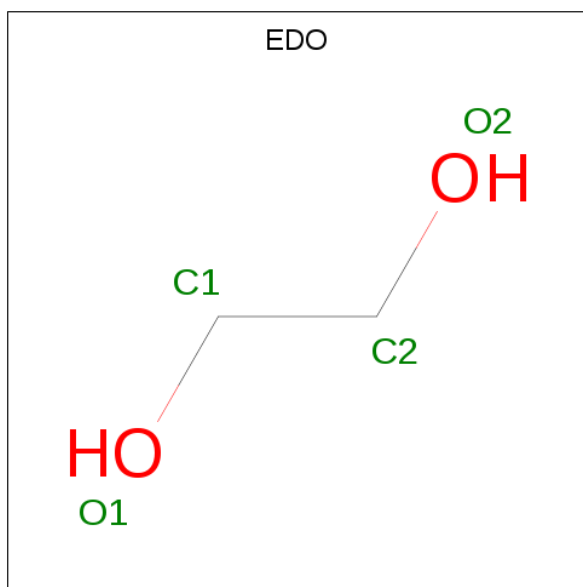
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

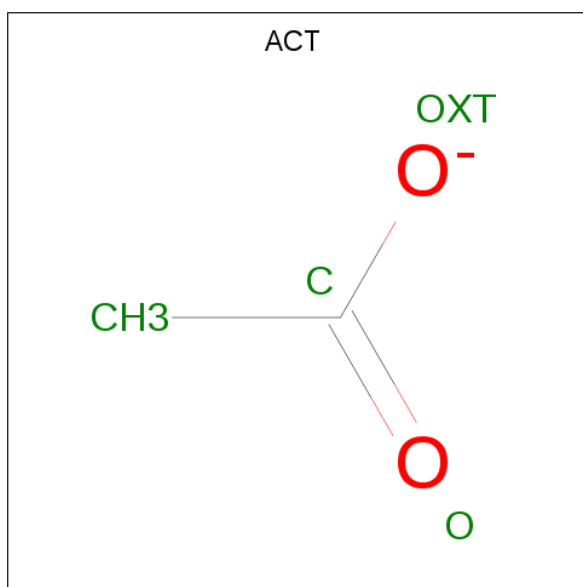
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

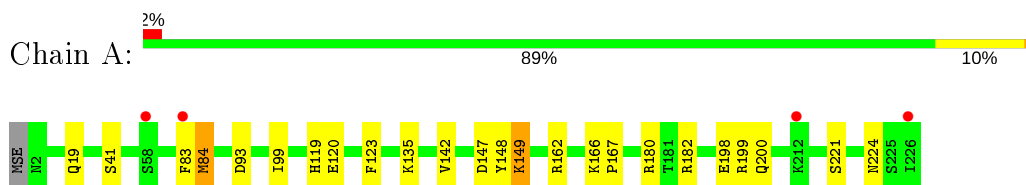
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	33	Total	O	0	0
			33	33		
7	C	35	Total	O	0	0
			35	35		
7	D	38	Total	O	0	0
			38	38		
7	H	11	Total	O	0	0
			11	11		
7	I	14	Total	O	0	0
			14	14		
7	J	15	Total	O	0	0
			15	15		
7	K	13	Total	O	0	0
			13	13		

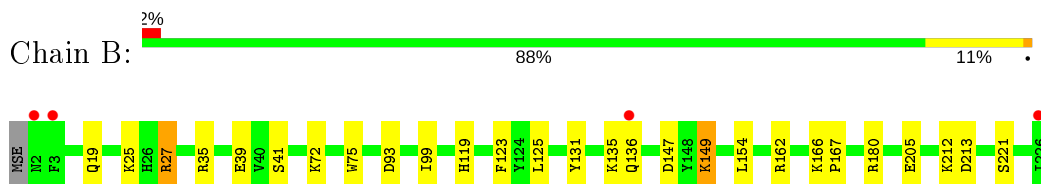
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

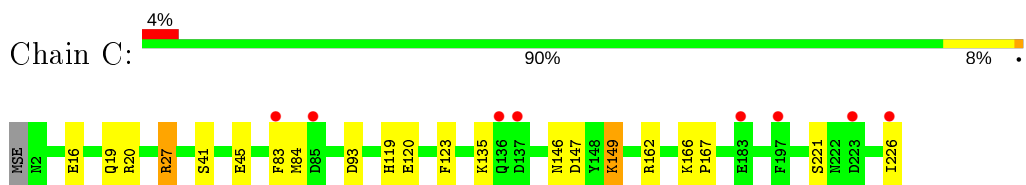
- Molecule 1: R-SwaI protein



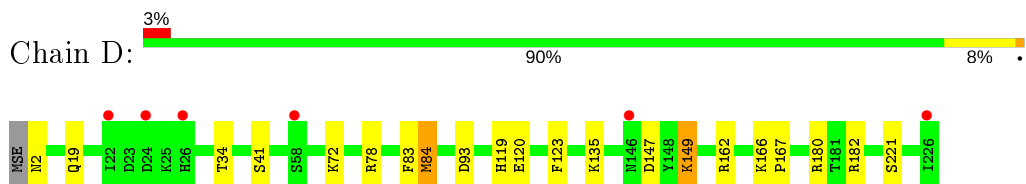
- Molecule 1: R-SwaI protein



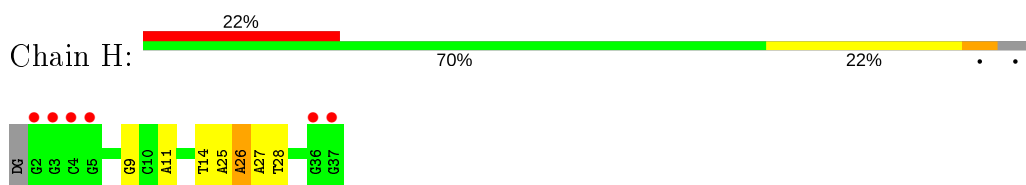
- Molecule 1: R-SwaI protein



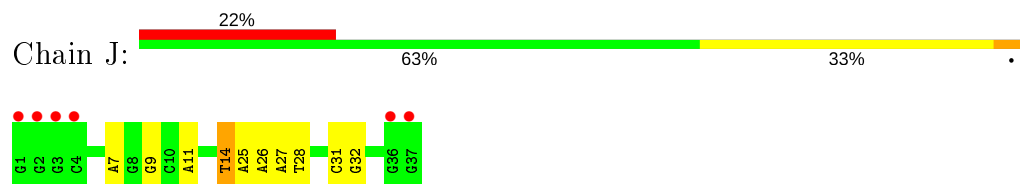
- Molecule 1: R-SwaI protein



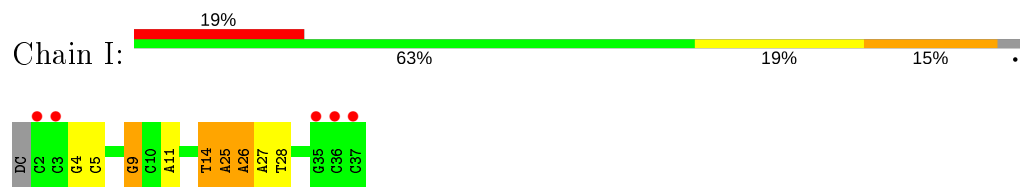
- Molecule 2: DNA (26-MER)



- Molecule 2: DNA (26-MER)



● Molecule 3: DNA (26-MER)



● Molecule 3: DNA (26-MER)



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.86 Å 57.06 Å 112.78 Å 90.00° 108.22° 90.00°	Depositor
Resolution (Å)	49.00 – 2.30 48.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.00-2.30) 95.3 (48.21-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.29 Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.198 , 0.242 0.205 , 0.245	Depositor DCC
R_{free} test set	2971 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3203e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, ACT

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	1.03	3/1932 (0.2%)	1.00	6/2587 (0.2%)
1	B	1.00	3/1932 (0.2%)	1.03	7/2587 (0.3%)
1	C	0.99	3/1945 (0.2%)	1.00	3/2605 (0.1%)
1	D	0.96	2/1932 (0.1%)	0.97	5/2587 (0.2%)
2	H	0.98	3/654 (0.5%)	1.56	13/1009 (1.3%)
2	J	1.15	2/676 (0.3%)	1.18	7/1044 (0.7%)
3	I	0.81	0/629	1.42	12/967 (1.2%)
3	K	1.99	4/629 (0.6%)	1.28	7/967 (0.7%)
All	All	1.08	20/10329 (0.2%)	1.11	60/14353 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	K	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	25[A]	DA	C6-N6	-31.06	1.09	1.33
3	K	25[B]	DA	C6-N6	-31.06	1.09	1.33
2	J	14[A]	DT	O3'-P	-16.39	1.41	1.61
2	J	14[B]	DT	O3'-P	-16.39	1.41	1.61
3	K	14[A]	DT	O3'-P	11.32	1.74	1.61
3	K	14[B]	DT	O3'-P	11.32	1.74	1.61
2	H	14[A]	DT	O3'-P	10.49	1.73	1.61
2	H	14[B]	DT	O3'-P	10.49	1.73	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	GLU	CD-OE1	7.33	1.33	1.25
1	C	147[A]	ASP	CB-CG	6.54	1.65	1.51
1	C	147[B]	ASP	CB-CG	6.54	1.65	1.51
1	B	147	ASP	CB-CG	6.42	1.65	1.51
1	B	39	GLU	CD-OE1	6.21	1.32	1.25
1	C	45	GLU	CG-CD	5.71	1.60	1.51
1	D	147	ASP	CB-CG	5.67	1.63	1.51
1	A	120	GLU	CD-OE1	5.45	1.31	1.25
1	A	147[A]	ASP	CB-CG	5.41	1.63	1.51
1	A	147[B]	ASP	CB-CG	5.41	1.63	1.51
2	H	26	DA	O3'-P	-5.38	1.54	1.61
1	B	75	TRP	CB-CG	5.32	1.59	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	25[A]	DA	O5'-P-OP2	-17.32	89.91	110.70
2	H	25[B]	DA	O5'-P-OP2	-17.32	89.91	110.70
2	H	14[A]	DT	OP2-P-O3'	12.69	133.11	105.20
2	H	14[B]	DT	OP2-P-O3'	12.69	133.11	105.20
3	I	14[A]	DT	OP2-P-O3'	-12.27	78.21	105.20
3	I	14[B]	DT	OP2-P-O3'	-12.27	78.21	105.20
2	H	25[A]	DA	O5'-P-OP1	10.37	123.14	110.70
2	H	25[B]	DA	O5'-P-OP1	10.37	123.14	110.70
3	K	25[A]	DA	O5'-P-OP1	10.25	123.00	110.70
3	K	25[B]	DA	O5'-P-OP1	10.25	123.00	110.70
2	H	14[A]	DT	P-O3'-C3'	-9.52	108.28	119.70
2	H	14[B]	DT	P-O3'-C3'	-9.52	108.28	119.70
3	I	9	DG	O5'-P-OP2	-9.43	97.22	105.70
2	H	9	DG	O5'-P-OP2	-8.04	98.47	105.70
2	J	9	DG	O5'-P-OP2	-7.93	98.56	105.70
2	J	14[A]	DT	OP1-P-O3'	-7.87	87.89	105.20
2	J	14[B]	DT	OP1-P-O3'	-7.87	87.89	105.20
1	A	84	MSE	CG-SE-CE	-7.49	82.42	98.90
3	K	9	DG	O5'-P-OP2	-7.39	99.05	105.70
3	I	14[A]	DT	P-O3'-C3'	7.37	128.54	119.70
3	I	14[B]	DT	P-O3'-C3'	7.37	128.54	119.70
1	B	213	ASP	CB-CG-OD2	-7.31	111.72	118.30
3	I	25[A]	DA	O5'-P-OP2	7.03	119.13	110.70
3	I	25[B]	DA	O5'-P-OP2	7.03	119.13	110.70
3	I	28	DT	O5'-P-OP2	-6.89	99.50	105.70
2	J	28	DT	O5'-P-OP2	-6.84	99.55	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	93	ASP	CB-CG-OD1	6.76	124.39	118.30
2	H	14[A]	DT	OP1-P-O3'	-6.71	90.44	105.20
2	H	14[B]	DT	OP1-P-O3'	-6.71	90.44	105.20
1	D	84	MSE	CG-SE-CE	-6.47	84.66	98.90
1	C	93	ASP	CB-CG-OD1	6.43	124.09	118.30
2	J	11	DA	O5'-P-OP2	-6.38	99.96	105.70
1	C	120	GLU	CA-CB-CG	6.26	127.18	113.40
1	B	93	ASP	CB-CG-OD1	6.09	123.78	118.30
2	J	14[A]	DT	OP2-P-O3'	5.80	117.96	105.20
2	J	14[B]	DT	OP2-P-O3'	5.80	117.96	105.20
1	B	25	LYS	CB-CA-C	5.80	122.00	110.40
3	K	28	DT	O5'-P-OP1	5.76	117.62	110.70
1	D	180	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	35	ARG	NE-CZ-NH1	5.63	123.11	120.30
3	I	25[A]	DA	O5'-P-OP1	5.54	117.34	110.70
3	I	25[B]	DA	O5'-P-OP1	5.54	117.34	110.70
1	B	180	ARG	NE-CZ-NH1	5.53	123.07	120.30
3	I	28	DT	O5'-P-OP1	5.50	117.30	110.70
1	A	224	ASN	CB-CA-C	-5.38	99.65	110.40
2	H	28	DT	O5'-P-OP1	5.37	117.15	110.70
1	C	27	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	B	27	ARG	C-N-CD	5.27	139.46	128.40
1	A	199	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	K	25[A]	DA	C1'-O4'-C4'	-5.19	104.91	110.10
3	K	25[B]	DA	C1'-O4'-C4'	-5.19	104.91	110.10
1	A	180	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	H	11	DA	O5'-P-OP2	-5.13	101.08	105.70
1	B	27	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	182	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	182	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	78	ARG	NE-CZ-NH2	-5.03	117.79	120.30
3	I	11	DA	O5'-P-OP2	-5.02	101.18	105.70
3	K	11	DA	O5'-P-OP2	-5.01	101.19	105.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	26	DA	Sidechain
3	K	25[A]	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	A	1894	0	1873	10	1
1	B	1891	0	1876	8	2
1	C	1904	0	1878	6	1
1	D	1894	0	1875	8	0
2	H	582	0	315	1	0
2	J	601	0	327	5	0
3	I	563	0	317	5	0
3	K	563	0	315	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	24	2	0
5	D	4	0	6	0	0
5	H	4	0	6	0	0
6	B	4	0	3	0	0
7	A	53	0	0	2	0
7	B	33	0	0	1	0
7	C	35	0	0	0	0
7	D	38	0	0	3	0
7	H	11	0	0	0	0
7	I	14	0	0	0	0
7	J	15	0	0	0	0
7	K	13	0	0	1	0
All	All	10136	0	8815	48	2

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 3.

All (48) 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:J:14[B]:DT:O3'	2:J:25[B]:DA:P	2.45	0.74
2:J:7:DA:N6	3:K:32:DT:O4	2.18	0.72
1:C:119:HIS:HD2	1:D:221:SER:OG	1.76	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:14[B]:DT:C2'	3:K:25[B]:DA:H5''	2.23	0.67
3:I:14[B]:DT:O3'	3:I:25[B]:DA:OP1	2.13	0.66
1:A:83:PHE:CD2	1:A:84:MSE:HG3	2.31	0.66
1:A:119:HIS:HD2	1:B:221:SER:OG	1.79	0.65
1:A:221:SER:OG	1:B:119:HIS:HD2	1.79	0.64
1:A:200:GLN:NE2	7:A:401:HOH:O	2.32	0.62
1:D:83:PHE:CD2	1:D:84:MSE:HG3	2.36	0.60
1:A:99:ILE:CD1	1:A:142:VAL:HG21	2.33	0.59
1:C:83:PHE:CD2	1:C:84:MSE:HG3	2.36	0.59
1:C:221:SER:OG	1:D:119:HIS:HD2	1.89	0.55
3:K:14[B]:DT:H2''	3:K:25[B]:DA:H5''	1.90	0.53
2:J:26:DA:H5'	7:K:110:HOH:O	2.09	0.53
1:A:99:ILE:HD13	1:A:142:VAL:HG21	1.91	0.53
1:A:99:ILE:HD13	1:A:142:VAL:CG2	2.40	0.52
1:D:84:MSE:SE	7:D:433:HOH:O	2.77	0.52
2:J:26:DA:C2	2:J:27:DA:C4	3.00	0.50
1:D:34:THR:O	7:D:401:HOH:O	2.19	0.49
2:H:26:DA:C2	2:H:27:DA:C4	3.01	0.49
5:A:304:EDO:H22	7:A:427:HOH:O	2.12	0.48
3:I:14[B]:DT:O3'	3:I:25[B]:DA:P	2.72	0.48
5:A:304:EDO:H12	3:I:9:DG:H2'	1.95	0.48
3:K:13:DT:H2''	3:K:14[B]:DT:O5'	2.13	0.48
1:A:166:LYS:N	1:A:167:PRO:HA	2.29	0.48
1:B:72:LYS:NZ	7:B:402:HOH:O	2.46	0.47
3:I:26:DA:C2	3:I:27:DA:C4	3.03	0.47
1:C:166:LYS:N	1:C:167:PRO:HA	2.30	0.46
1:B:99:ILE:HD12	1:B:99:ILE:C	2.36	0.46
1:D:72:LYS:NZ	7:D:405:HOH:O	2.48	0.46
1:C:16:GLU:O	1:C:20:ARG:HG2	2.16	0.45
1:A:99:ILE:HD11	1:A:142:VAL:HG21	1.99	0.45
3:I:4:DG:H2''	3:I:5:DC:OP2	2.17	0.45
1:C:19:GLN:OE1	1:C:149:LYS:NZ	2.50	0.45
2:J:31:DC:H2''	2:J:32:DG:C8	2.52	0.45
1:A:19:GLN:OE1	1:A:149:LYS:NZ	2.50	0.44
1:B:19:GLN:OE1	1:B:149:LYS:NZ	2.51	0.44
1:B:166:LYS:N	1:B:167:PRO:HA	2.34	0.43
3:K:3:DC:H4'	3:K:4:DG:OP1	2.19	0.42
3:K:14[B]:DT:H2'	3:K:25[B]:DA:H5''	1.98	0.42
1:D:19:GLN:OE1	1:D:149:LYS:NZ	2.53	0.42
3:K:14[B]:DT:C2'	3:K:25[B]:DA:C5'	2.95	0.42
3:K:26:DA:C2	3:K:27:DA:C4	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:LYS:N	1:D:167:PRO:HA	2.36	0.41
3:K:2:DC:H2'	3:K:3:DC:C5	2.55	0.41
1:B:99:ILE:CG2	1:B:131:TYR:HB3	2.50	0.41
1:B:125:LEU:HD23	1:B:154:LEU:HD22	2.03	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:NZ	1:C:146:ASN:O[2_546]	2.10	0.10
1:A:148:TYR:OH	1:B:205:GLU:OE2[1_565]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/226 (99%)	216 (96%)	8 (4%)	0	100	100
1	B	224/226 (99%)	216 (96%)	8 (4%)	0	100	100
1	C	226/226 (100%)	219 (97%)	7 (3%)	0	100	100
1	D	224/226 (99%)	217 (97%)	7 (3%)	0	100	100
All	All	898/904 (99%)	868 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/206 (102%)	204 (97%)	6 (3%)	42	58
1	B	210/206 (102%)	203 (97%)	7 (3%)	38	53
1	C	211/206 (102%)	204 (97%)	7 (3%)	38	53
1	D	210/206 (102%)	204 (97%)	6 (3%)	42	58
All	All	841/824 (102%)	815 (97%)	26 (3%)	40	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	123	PHE
1	A	135	LYS
1	A	149	LYS
1	A	162	ARG
1	A	198	GLU
1	B	27	ARG
1	B	41	SER
1	B	123	PHE
1	B	135	LYS
1	B	136	GLN
1	B	149	LYS
1	B	162	ARG
1	C	27	ARG
1	C	41	SER
1	C	123	PHE
1	C	135	LYS
1	C	149	LYS
1	C	162	ARG
1	C	226	ILE
1	D	2	ASN
1	D	41	SER
1	D	123	PHE
1	D	135	LYS
1	D	149	LYS
1	D	162	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	187	HIS
1	A	200	GLN
1	B	119	HIS
1	B	200	GLN
1	C	119	HIS
1	C	187	HIS
1	D	101	ASN
1	D	119	HIS
1	D	146	ASN
1	D	187	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	EDO	A	302	-	3,3,3	0.59	0	2,2,2	0.49	0
5	EDO	D	302	-	3,3,3	0.61	0	2,2,2	0.23	0
6	ACT	B	302	-	1,3,3	1.92	0	0,3,3	0.00	-
5	EDO	A	305	-	3,3,3	0.55	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	304	-	3,3,3	1.16	0	2,2,2	0.96	0
5	EDO	H	101	-	3,3,3	0.72	0	2,2,2	0.55	0
5	EDO	A	303	-	3,3,3	0.68	0	2,2,2	0.37	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	EDO	A	302	-	-	0/1/1/1	-
5	EDO	D	302	-	-	1/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	A	304	-	-	1/1/1/1	-
5	EDO	H	101	-	-	0/1/1/1	-
5	EDO	A	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	302	EDO	O1-C1-C2-O2
5	A	304	EDO	O1-C1-C2-O2
5	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	EDO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
2	J	1
3	I	1
3	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	14[B]:DT	O3'	25[B]:DA	P	3.50
1	K	14[B]:DT	O3'	25[B]:DA	P	2.83
1	I	14[B]:DT	O3'	25[B]:DA	P	2.72
1	J	14[B]:DT	O3'	25[B]:DA	P	2.45

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	221/226 (97%)	0.15	4 (1%) 68 74	30, 53, 93, 121	0
1	B	221/226 (97%)	0.07	4 (1%) 68 74	39, 62, 92, 117	0
1	C	221/226 (97%)	0.24	8 (3%) 42 49	38, 65, 100, 126	0
1	D	221/226 (97%)	0.19	6 (2%) 54 62	35, 60, 99, 133	0
2	H	26/27 (96%)	0.88	6 (23%) 0 1	32, 81, 198, 226	0
2	J	27/27 (100%)	1.13	6 (22%) 0 1	37, 80, 191, 215	0
3	I	26/27 (96%)	0.91	5 (19%) 1 1	35, 78, 192, 215	0
3	K	26/27 (96%)	0.90	6 (23%) 0 1	35, 78, 185, 214	0
All	All	989/1012 (97%)	0.25	45 (4%) 32 39	30, 61, 111, 226	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	1	DG	9.0
2	H	2	DG	8.3
3	I	37	DC	7.4
1	A	226	ILE	6.6
2	J	2	DG	5.8
3	K	2	DC	5.6
1	D	226	ILE	5.6
1	C	226	ILE	5.5
3	K	37	DC	5.3
3	I	2	DC	5.2
2	J	37	DG	5.1
2	H	3	DG	4.8
3	K	3	DC	4.8
3	I	35	DG	3.7
3	K	4	DG	3.6
2	J	36	DG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	4	DC	3.5
1	B	226	ILE	3.4
1	D	24	ASP	3.3
2	H	37	DG	3.3
1	B	2	ASN	3.2
2	J	3	DG	3.2
2	H	36	DG	3.1
1	B	3	PHE	3.1
1	C	85	ASP	3.0
3	I	36	DC	3.0
1	D	146	ASN	3.0
1	D	22	ILE	2.9
1	C	136	GLN	2.9
3	K	35	DG	2.8
1	B	136	GLN	2.7
1	D	26	HIS	2.7
1	C	197	PHE	2.6
1	C	137	ASP	2.6
2	J	4	DC	2.5
3	K	36	DC	2.4
2	H	5	DG	2.3
1	C	183	GLU	2.3
1	A	83	PHE	2.3
1	C	223[A]	ASP	2.3
1	D	58	SER	2.3
3	I	3	DC	2.2
1	C	83	PHE	2.1
1	A	58	SER	2.1
1	A	212	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
5	EDO	A	304	4/4	0.56	0.38	55,58,61,64	0
5	EDO	D	302	4/4	0.64	0.24	66,75,77,79	0
5	EDO	A	303	4/4	0.77	0.24	70,74,74,76	0
5	EDO	A	302	4/4	0.89	0.24	59,60,60,62	0
5	EDO	H	101	4/4	0.91	0.23	48,52,55,56	0
5	EDO	A	305	4/4	0.91	0.12	69,75,75,76	0
6	ACT	B	302	4/4	0.92	0.14	80,81,83,88	0
4	CA	C	301	1/1	0.97	0.11	51,51,51,51	0
4	CA	A	301	1/1	0.98	0.16	42,42,42,42	0
4	CA	D	301	1/1	0.99	0.16	51,51,51,51	0
4	CA	B	301	1/1	0.99	0.16	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.