



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:51 am BST

PDB ID : 3GYH  
Title : Crystal Structure Analysis of S. Pombe ATL in complex with damaged DNA containing POB  
Authors : Tubbs, J.L.; Arvai, A.S.; Tainer, J.A.; Shin, D.S.  
Deposited on : 2009-04-03  
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](mailto: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

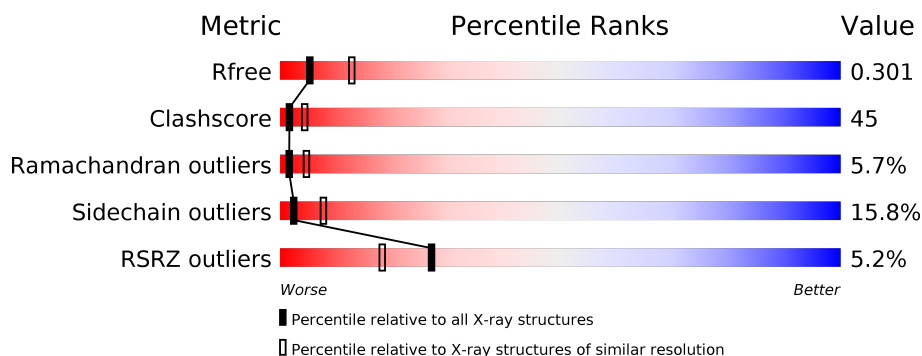
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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	X	116	<div> <div>6%</div> <div>42%</div> <div>36%</div> <div>12%</div> <div>•</div> <div>7%</div> </div>
2	Y	13	<div> <div>8%</div> <div>77%</div> <div>15%</div> </div>
3	Z	13	<div> <div>15%</div> <div>54%</div> <div>31%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PBO	Y	200	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1430 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 Alkyltransferase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	108	Total	C	N	O	S	0	0	0
			890	563	156	165	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	109	GLY	-	EXPRESSION TAG	UNP Q9UTN9
X	110	SER	-	EXPRESSION TAG	UNP Q9UTN9
X	111	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	112	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	113	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	114	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	115	HIS	-	EXPRESSION TAG	UNP Q9UTN9
X	116	HIS	-	EXPRESSION TAG	UNP Q9UTN9

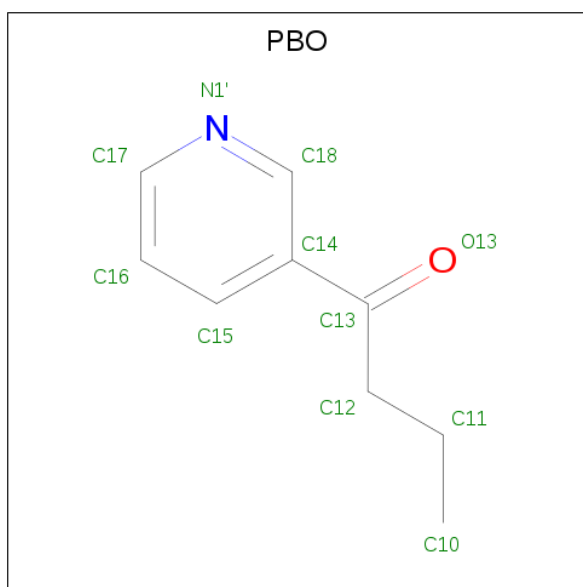
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*CP\*AP\*TP\*GP\*GP\*CP\*TP\*AP\*GP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*TP\*AP\*CP\*TP\*AP\*GP\*CP\*CP\*AP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is 1-PYRIDIN-3-YLBUTAN-1-ONE (three-letter code: PBO) (formula: C<sub>9</sub>H<sub>11</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Y	1	Total	C	N	O	0	0
			11	9	1	1		

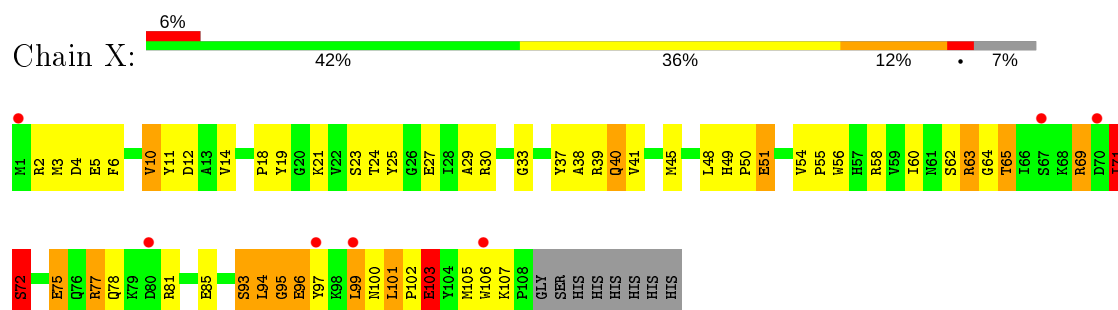
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	2	Total	O	0	0
			2	2		

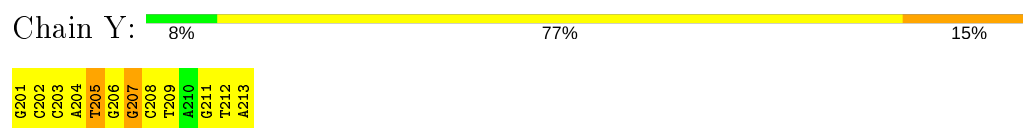
### 3 Residue-property plots

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.

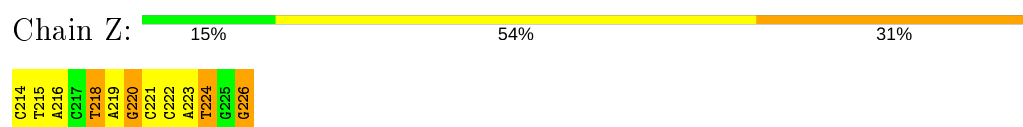
- Molecule 1: Alkyltransferase-like protein 1



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



- Molecule 3: DNA (5'-D(\*CP\*TP\*AP\*CP\*TP\*AP\*GP\*CP\*CP\*AP\*TP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.18 Å 60.18 Å 235.55 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.94 – 2.80 31.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (34.94-2.80) 88.2 (31.36-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.44 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.285 0.239 , 0.301	Depositor DCC
$R_{free}$ test set	341 reflections (5.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 91.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	X	0.43	0/913	0.53	0/1232
2	Y	1.45	6/297 (2.0%)	2.61	20/457 (4.4%)
3	Z	0.78	0/293	1.55	5/450 (1.1%)
All	All	0.80	6/1503 (0.4%)	1.46	25/2139 (1.2%)

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	X	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	207	DG	C6-O6	15.01	1.37	1.24
2	Y	207	DG	C8-N7	9.12	1.36	1.30
2	Y	207	DG	C6-N1	-6.43	1.35	1.39
2	Y	207	DG	N7-C5	-6.40	1.35	1.39
2	Y	207	DG	N9-C8	-5.70	1.33	1.37
2	Y	207	DG	N9-C4	-5.65	1.33	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	207	DG	N3-C4-C5	-18.36	119.42	128.60
2	Y	207	DG	C2-N3-C4	15.62	119.71	111.90
2	Y	206	DG	OP2-P-O3'	15.43	139.15	105.20
2	Y	207	DG	C5-C6-N1	14.27	118.63	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	207	DG	C5-C6-O6	-13.59	120.44	128.60
2	Y	206	DG	OP1-P-O3'	-12.45	77.81	105.20
2	Y	207	DG	P-O3'-C3'	-10.69	106.87	119.70
2	Y	207	DG	C4-C5-N7	-10.66	106.54	110.80
2	Y	207	DG	N3-C4-N9	10.44	132.26	126.00
2	Y	207	DG	OP2-P-O3'	9.71	126.57	105.20
2	Y	207	DG	N7-C8-N9	-8.89	108.65	113.10
2	Y	207	DG	C6-N1-C2	-8.11	120.24	125.10
2	Y	207	DG	N9-C4-C5	7.28	108.31	105.40
2	Y	207	DG	C5-N7-C8	7.25	107.92	104.30
2	Y	207	DG	OP1-P-O3'	-7.24	89.26	105.20
3	Z	226	DG	O4'-C4'-C3'	-7.01	101.69	104.50
2	Y	206	DG	P-O3'-C3'	-6.95	111.36	119.70
3	Z	224	DT	N3-C4-O4	6.81	123.99	119.90
3	Z	218	DT	O4'-C1'-N1	6.53	112.57	108.00
2	Y	205	DT	O4'-C1'-N1	-6.01	103.80	108.00
2	Y	211	DG	O4'-C1'-N9	5.95	112.16	108.00
3	Z	220	DG	P-O3'-C3'	-5.89	112.64	119.70
3	Z	224	DT	C5-C4-O4	-5.68	120.93	124.90
2	Y	207	DG	C8-N9-C4	5.42	108.57	106.40
2	Y	207	DG	C6-C5-N7	5.00	133.40	130.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	93	SER	Peptide

## 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	X	890	0	868	76	1
2	Y	265	0	148	22	0
3	Z	262	0	148	29	0
4	Y	11	0	10	7	0
5	X	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1430	0	1174	115	1

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 45.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:221:DC:H2''	3:Z:222:DC:H5'	1.27	1.17
3:Z:220:DG:H2''	3:Z:221:DC:H5'	1.31	1.13
2:Y:209:DT:H3	3:Z:219:DA:H62	1.09	0.96
1:X:18:PRO:HG2	1:X:21:LYS:HB2	1.46	0.95
3:Z:219:DA:H2''	3:Z:220:DG:H5''	1.52	0.92
1:X:39:ARG:NH2	3:Z:221:DC:N3	2.17	0.92
1:X:25:TYR:CD1	2:Y:208:DC:H5''	2.09	0.86
2:Y:208:DC:H2''	2:Y:209:DT:H5'	1.58	0.85
1:X:71:ILE:HG23	1:X:71:ILE:O	1.74	0.85
2:Y:201:DG:H2''	2:Y:202:DC:O5'	1.75	0.83
3:Z:220:DG:C2'	3:Z:221:DC:H5'	2.09	0.80
3:Z:214:DC:H2'	3:Z:215:DT:C6	2.16	0.80
2:Y:202:DC:H2''	2:Y:203:DC:OP2	1.83	0.79
3:Z:218:DT:C2'	3:Z:219:DA:H5''	2.14	0.78
1:X:40:GLN:NE2	1:X:40:GLN:H	1.82	0.76
3:Z:226:DG:C8	3:Z:226:DG:H5'	2.19	0.76
1:X:64:GLY:HA2	1:X:101:LEU:CD2	2.15	0.75
1:X:71:ILE:CG2	1:X:71:ILE:O	2.33	0.75
1:X:64:GLY:HA2	1:X:101:LEU:HD23	1.69	0.75
3:Z:221:DC:H2''	3:Z:222:DC:C5'	2.16	0.69
3:Z:218:DT:C3'	3:Z:219:DA:H5''	2.23	0.68
1:X:24:THR:HG22	1:X:27:GLU:HB2	1.75	0.68
2:Y:212:DT:H1'	2:Y:213:DA:H5'	1.76	0.67
3:Z:226:DG:H8	3:Z:226:DG:H5'	1.60	0.66
3:Z:218:DT:H2'	3:Z:219:DA:N3	2.12	0.65
1:X:23:SER:OG	1:X:24:THR:N	2.31	0.64
1:X:45:MET:O	4:Y:200:PBO:H102	1.97	0.64
1:X:77:ARG:HG3	4:Y:200:PBO:H16	1.79	0.64
2:Y:204:DA:H2'	2:Y:204:DA:O5'	1.98	0.64
1:X:24:THR:HG23	1:X:27:GLU:H	1.63	0.63
1:X:55:PRO:HB2	1:X:58:ARG:HD2	1.81	0.61
1:X:75:GLU:O	1:X:78:GLN:N	2.33	0.61
1:X:2:ARG:NH1	1:X:4:ASP:OD1	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:220:DG:H2''	3:Z:221:DC:C5'	2.20	0.60
1:X:29:ALA:HB2	1:X:41:VAL:HG21	1.84	0.60
1:X:11:TYR:CE2	1:X:48:LEU:HD21	2.35	0.60
1:X:2:ARG:HB3	1:X:4:ASP:OD2	2.01	0.59
1:X:95:GLY:O	1:X:96:GLU:C	2.39	0.59
1:X:56:TRP:CD2	4:Y:200:PBO:H111	2.36	0.59
2:Y:202:DC:H1'	2:Y:203:DC:H5'	1.85	0.59
3:Z:223:DA:H2''	3:Z:224:DT:H5'	1.86	0.58
1:X:95:GLY:O	1:X:97:TYR:N	2.37	0.58
1:X:100:ASN:OD1	1:X:103:GLU:HB2	2.04	0.58
1:X:25:TYR:CE1	2:Y:208:DC:H5''	2.38	0.58
3:Z:221:DC:C2'	3:Z:222:DC:H5'	2.17	0.58
1:X:30:ARG:HH11	1:X:30:ARG:HG3	1.69	0.58
1:X:29:ALA:HB2	1:X:41:VAL:CG2	2.33	0.58
1:X:64:GLY:O	1:X:99:LEU:HD13	2.04	0.58
1:X:37:TYR:OH	3:Z:223:DA:OP1	2.21	0.58
1:X:14:VAL:O	1:X:55:PRO:HG2	2.03	0.57
1:X:50:PRO:HA	4:Y:200:PBO:H18	1.86	0.56
1:X:64:GLY:CA	1:X:101:LEU:HD23	2.35	0.56
1:X:71:ILE:O	1:X:72:SER:O	2.25	0.55
1:X:2:ARG:HB2	1:X:5:GLU:HG3	1.88	0.55
1:X:30:ARG:NH1	1:X:30:ARG:HG3	2.22	0.55
1:X:55:PRO:CB	1:X:58:ARG:HD2	2.37	0.55
1:X:77:ARG:HD3	4:Y:200:PBO:H17	1.88	0.55
1:X:56:TRP:CE3	4:Y:200:PBO:H111	2.42	0.54
2:Y:201:DG:H8	2:Y:201:DG:H5'	1.72	0.54
1:X:19:TYR:CZ	1:X:85:GLU:HA	2.42	0.54
1:X:25:TYR:CZ	2:Y:207:DG:H2''	2.43	0.53
1:X:3:MET:HE1	3:Z:223:DA:H4'	1.90	0.53
2:Y:212:DT:H5'	2:Y:212:DT:H6	1.74	0.53
1:X:75:GLU:HG2	1:X:75:GLU:O	2.08	0.52
3:Z:216:DA:OP2	3:Z:216:DA:H2'	2.09	0.52
2:Y:209:DT:C4	3:Z:219:DA:N6	2.77	0.52
1:X:11:TYR:CZ	1:X:48:LEU:HD21	2.44	0.52
3:Z:218:DT:H2'	3:Z:219:DA:C2	2.45	0.52
1:X:64:GLY:HA2	1:X:101:LEU:HD22	1.91	0.52
1:X:94:LEU:C	1:X:96:GLU:H	2.14	0.51
1:X:3:MET:CE	3:Z:223:DA:H4'	2.40	0.51
1:X:45:MET:HA	1:X:48:LEU:HD12	1.94	0.50
1:X:40:GLN:HE21	1:X:40:GLN:H	1.59	0.50
1:X:81:ARG:O	1:X:85:GLU:HG2	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:63:ARG:CZ	1:X:63:ARG:HB3	2.43	0.49
1:X:54:VAL:CG1	1:X:55:PRO:CD	2.91	0.49
1:X:54:VAL:CG1	1:X:55:PRO:HD2	2.43	0.48
2:Y:208:DC:C2'	2:Y:209:DT:H5'	2.36	0.48
1:X:94:LEU:O	1:X:96:GLU:N	2.45	0.48
1:X:40:GLN:NE2	1:X:40:GLN:N	2.58	0.48
1:X:39:ARG:HD2	3:Z:221:DC:O2	2.15	0.47
1:X:77:ARG:HG3	4:Y:200:PBO:C16	2.44	0.47
2:Y:201:DG:C8	2:Y:201:DG:H5'	2.50	0.47
1:X:5:GLU:O	1:X:6:PHE:C	2.54	0.46
1:X:60:ILE:HB	1:X:65:THR:O	2.15	0.46
2:Y:204:DA:O5'	2:Y:204:DA:C2'	2.55	0.46
1:X:25:TYR:HB2	2:Y:209:DT:OP1	2.16	0.46
3:Z:214:DC:H2''	3:Z:215:DT:H5'	1.98	0.45
1:X:54:VAL:HG13	1:X:55:PRO:CD	2.46	0.45
1:X:24:THR:O	1:X:25:TYR:C	2.56	0.44
1:X:54:VAL:HG13	1:X:55:PRO:HD2	1.99	0.44
1:X:65:THR:HB	1:X:97:TYR:O	2.18	0.44
3:Z:214:DC:H2'	3:Z:215:DT:H6	1.76	0.44
2:Y:212:DT:H5'	2:Y:212:DT:C6	2.53	0.44
1:X:101:LEU:HB3	1:X:102:PRO:HD3	2.01	0.43
1:X:99:LEU:HD22	1:X:99:LEU:C	2.37	0.43
3:Z:219:DA:H2''	3:Z:220:DG:C5'	2.34	0.43
1:X:106:TRP:C	1:X:107:LYS:HG3	2.40	0.43
1:X:10:VAL:O	1:X:14:VAL:HG23	2.19	0.42
1:X:49:HIS:HB3	1:X:51:GLU:OE1	2.19	0.42
2:Y:204:DA:H1'	2:Y:205:DT:H5'	2.02	0.42
3:Z:223:DA:C2'	3:Z:224:DT:H5'	2.48	0.42
1:X:37:TYR:HA	1:X:40:GLN:NE2	2.34	0.42
1:X:75:GLU:C	1:X:77:ARG:N	2.72	0.42
1:X:30:ARG:O	1:X:33:GLY:N	2.42	0.42
1:X:69:ARG:CZ	1:X:75:GLU:HB2	2.50	0.42
1:X:37:TYR:O	1:X:41:VAL:HG23	2.19	0.41
1:X:62:SER:C	1:X:64:GLY:H	2.24	0.41
2:Y:203:DC:H2''	2:Y:204:DA:OP2	2.20	0.41
1:X:25:TYR:CD1	2:Y:208:DC:C5'	2.93	0.41
3:Z:218:DT:H2''	3:Z:219:DA:H5''	1.99	0.41
1:X:24:THR:CG2	1:X:27:GLU:HB2	2.49	0.40
1:X:38:ALA:O	1:X:39:ARG:C	2.60	0.40
2:Y:203:DC:C4	2:Y:204:DA:N6	2.89	0.40
3:Z:214:DC:H3'	3:Z:215:DT:H71	2.03	0.40

All (1) 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:X:2:ARG:NH2	1:X:12:ASP:OD2[12_545]	2.11	0.09

## 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	X	106/116 (91%)	78 (74%)	22 (21%)	6 (6%)	<b>1</b> <b>5</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	72	SER
1	X	96	GLU
1	X	103	GLU
1	X	10	VAL
1	X	71	ILE
1	X	95	GLY

### 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	X	95/102 (93%)	80 (84%)	15 (16%)	<b>2</b> <b>8</b>

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	40	GLN
1	X	51	GLU
1	X	63	ARG
1	X	65	THR
1	X	69	ARG
1	X	71	ILE
1	X	72	SER
1	X	75	GLU
1	X	77	ARG
1	X	93	SER
1	X	94	LEU
1	X	99	LEU
1	X	101	LEU
1	X	103	GLU
1	X	105	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	40	GLN

### 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](#)

1 ligand 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	PBO	Y	200	2	11,11,11	0.66	0	13,13,13	1.62	4 (30%)

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	PBO	Y	200	2	-	3/7/7/7	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	Y	200	PBO	C12-C13-C14	2.78	122.98	119.13
4	Y	200	PBO	C17-N1'-C18	2.64	121.42	116.85
4	Y	200	PBO	O13-C13-C14	-2.51	117.18	120.74
4	Y	200	PBO	C14-C18-N1'	-2.00	120.53	123.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	200	PBO	C10-C11-C12-C13
4	Y	200	PBO	C11-C12-C13-C14
4	Y	200	PBO	C11-C12-C13-O13

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	200	PBO	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	108/116 (93%)	0.48	7 (6%) 18 11	49, 84, 104, 111	0
2	Y	13/13 (100%)	0.09	0 100 100	59, 74, 92, 94	0
3	Z	13/13 (100%)	-0.65	0 100 100	69, 85, 105, 106	0
All	All	134/142 (94%)	0.33	7 (5%) 27 18	49, 84, 104, 111	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	106	TRP	3.0
1	X	99	LEU	3.0
1	X	70	ASP	2.8
1	X	1	MET	2.5
1	X	80	ASP	2.5
1	X	97	TYR	2.5
1	X	67	SER	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, 95<sup>th</sup> 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	PBO	Y	200	11/11	0.80	0.58	61,65,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.