



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:57 AM BST

PDB ID : 6W3U  
Title : APE1 exonuclease substrate complex R237C  
Authors : Freudenthal, B.D.; Whitaker, A.M.  
Deposited on : 2020-03-09  
Resolution : 2.40 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.

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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 : 2.13.1  
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) : 2.13.1

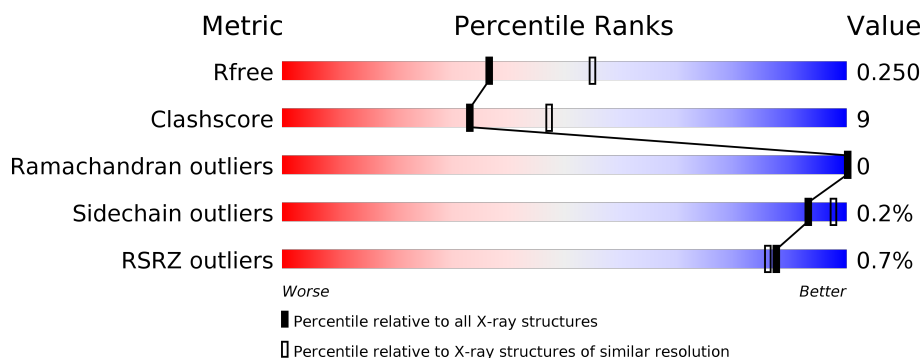
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	C	11	<div> <div>9%</div> <div>18%</div> <div>82%</div> </div>
2	D	11	<div> <div>64%</div> <div>18%</div> <div>18%</div> </div>
3	E	21	<div> <div>10%</div> <div>62%</div> <div>38%</div> </div>
4	A	276	<div> <div>89%</div> <div>11%</div> </div>
4	B	276	<div> <div>84%</div> <div>16%</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
2	C7R	D	10[A]	-	-	X	X
2	C7S	D	10[B]	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5408 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 DNA (5'-D(P\*TP\*CP\*GP\*AP\*CP\*GP\*GP\*AP\*TP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*(C7R))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	S	0	1	0
			222	106	41	63	10	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	21	Total	C	N	O	P	0	0	0
			426	203	79	124	20			

- Molecule 4 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	276	Total	C	N	O	S	0	1	0
			2185	1396	375	404	10			
4	B	276	Total	C	N	O	S	0	1	0
			2185	1398	376	401	10			

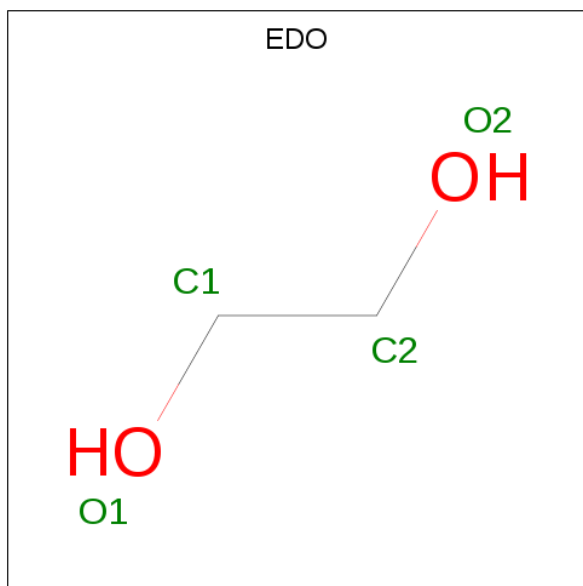
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	CYS	ARG	engineered mutation	UNP P27695
B	237	CYS	ARG	engineered mutation	UNP P27695

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

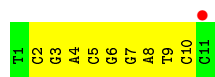
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total 2	O 2	0	0
9	E	10	Total 10	O 10	0	0
9	A	69	Total 69	O 69	0	0
9	B	73	Total 73	O 73	0	0

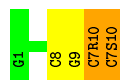
### 3 Residue-property plots [i](#)

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.

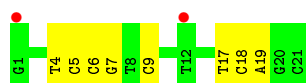
- Molecule 1: DNA (5'-D(P\*TP\*CP\*GP\*AP\*CP\*GP\*GP\*AP\*TP\*CP\*C)-3')



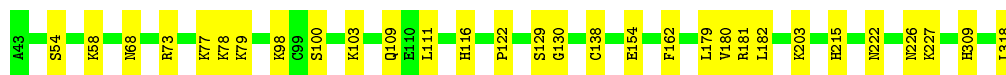
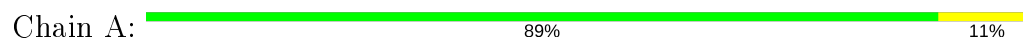
- Molecule 2: DNA (5'-D(\*GP\*CP\*TP\*GP\*AP\*TP\*GP\*CP\*GP\*(C7R))-3')



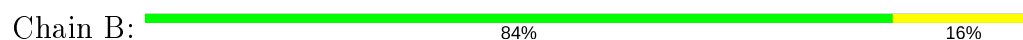
- Molecule 3: DNA (5'-D(\*GP\*GP\*AP\*TP\*CP\*CP\*GP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*CP\*AP\*TP\*CP\*AP\*GP\*C)-3')



- Molecule 4: DNA-(apurinic or apyrimidinic site) lyase



- Molecule 4: DNA-(apurinic or apyrimidinic site) lyase



R254	
Y262	
A263	
Y264	
T265	
K276	
R277	
V278	
G279	
W280	
R281	
F285	
R301	
H309	
G310	
P311	
I314	
I318	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.18Å 65.62Å 91.72Å 90.00° 110.52° 90.00°	Depositor
Resolution (Å)	46.76 – 2.40 46.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (46.76-2.40) 92.7 (46.76-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.184 , 0.250 0.184 , 0.250	Depositor DCC
$R_{free}$ test set	1441 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, C7S, C7R, EDO, CA

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	0.88	0/251	0.87	0/383
2	D	0.97	0/206	0.99	0/317
3	E	0.90	0/477	0.92	0/734
4	A	0.43	0/2246	0.60	0/3048
4	B	0.46	0/2246	0.61	0/3046
All	All	0.56	0/5426	0.68	0/7528

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	225	0	124	13	0
2	D	222	0	102	8	0
3	E	426	0	237	13	0
4	A	2185	0	2147	23	0
4	B	2185	0	2159	34	0
5	D	1	0	0	0	0
6	A	4	0	6	0	0
6	B	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	69	0	0	3	0
9	B	73	0	0	1	0
9	D	2	0	0	0	0
9	E	10	0	0	2	0
All	All	5408	0	4781	79	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 9.

All (79) 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:D:10[A]:C7R:SP2	4:B:171:TYR:OH	2.07	1.13
2:D:8:DC:H2"	2:D:9:DG:H5"	1.62	0.79
2:D:10[A]:C7R:C5'	9:B:502:HOH:O	2.35	0.74
1:C:4:DA:H2"	1:C:5:DC:H5"	1.70	0.73
4:A:162:PHE:O	4:A:203:LYS:NZ	2.25	0.69
4:A:54:SER:HB3	4:A:58:LYS:H	1.58	0.68
3:E:6:DC:H2"	3:E:7:DG:C8	2.28	0.68
4:B:150:GLU:CD	4:B:187:ARG:HH12	1.98	0.67
2:D:10[A]:C7R:C5	4:B:280:TRP:CZ2	2.78	0.67
3:E:17:DT:H5'	4:B:127:GLY:HA3	1.77	0.67
1:C:2:DC:H42	3:E:9:DC:H42	1.42	0.66
4:B:276:LYS:HB2	4:B:278:VAL:HG23	1.78	0.65
4:B:81:LEU:O	4:B:85:LYS:HG3	1.97	0.65
4:A:122:PRO:HB3	4:A:154:GLU:HA	1.79	0.64
4:B:150:GLU:OE1	4:B:187:ARG:NH1	2.30	0.64
4:B:179:LEU:HD21	4:B:228:LYS:O	2.01	0.60
2:D:10[A]:C7R:C3'	4:B:174:ASN:ND2	2.66	0.59
1:C:3:DG:H2'	1:C:4:DA:C8	2.37	0.59
4:B:202:ARG:HD2	6:B:401:EDO:H21	1.86	0.57
1:C:2:DC:H2"	1:C:3:DG:C8	2.40	0.56
1:C:2:DC:N4	3:E:9:DC:H42	2.03	0.56
3:E:4:DT:H2'	3:E:5:DC:C6	2.43	0.54
4:A:116:HIS:NE2	4:A:138:CYS:HB2	2.22	0.53
4:A:100:SER:OG	4:A:103:LYS:HG3	2.08	0.53
2:D:10[A]:C7R:O3'	4:B:212:ASN:OD1	2.27	0.52
4:A:54:SER:HB3	4:A:58:LYS:N	2.23	0.52
4:A:222:ASN:O	4:A:226:ASN:ND2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:215:HIS:HE1	9:A:564:HOH:O	1.93	0.51
3:E:5:DC:H2'	3:E:6:DC:C6	2.46	0.51
4:A:215:HIS:HD2	9:A:520:HOH:O	1.94	0.51
4:A:68:ASN:HB3	4:A:309:HIS:CG	2.47	0.49
4:B:172:VAL:O	4:B:212:ASN:ND2	2.44	0.49
1:C:4:DA:H61	3:E:7:DG:H1	1.60	0.49
4:B:262:TYR:HA	4:B:264:TYR:CZ	2.49	0.48
4:A:98:LYS:NZ	9:A:507:HOH:O	2.46	0.48
4:A:180:VAL:HG23	4:A:181:ARG:HG3	1.96	0.47
3:E:17:DT:H2''	3:E:18:DC:H5'	1.96	0.47
4:B:301:ARG:HB2	4:B:311:PRO:HG2	1.96	0.47
4:A:78:LYS:O	4:A:79:LYS:HB2	2.16	0.46
2:D:10[A]:C7R:C3'	4:B:174:ASN:HD21	2.29	0.45
4:B:67:TRP:CE2	4:B:311:PRO:HD3	2.52	0.45
1:C:6:DG:C6	1:C:7:DG:C6	3.05	0.45
4:A:116:HIS:CD2	4:A:138:CYS:HB2	2.52	0.45
1:C:7:DG:H2''	1:C:8:DA:O4'	2.17	0.44
1:C:6:DG:H2'	1:C:7:DG:C8	2.52	0.44
4:A:73:ARG:HH12	4:A:103:LYS:HD2	1.83	0.44
4:B:116:HIS:NE2	4:B:138:CYS:HB2	2.33	0.44
1:C:3:DG:H2''	1:C:4:DA:O4'	2.18	0.43
3:E:5:DC:H2'	3:E:6:DC:H6	1.83	0.43
4:B:68:ASN:HB3	4:B:309:HIS:CG	2.53	0.43
3:E:17:DT:H5''	4:B:126:GLU:HG2	1.99	0.43
4:B:196:LEU:HD22	4:B:205:LEU:HD21	2.00	0.43
4:B:254:ARG:HD3	4:B:254:ARG:HA	1.82	0.43
4:B:77:LYS:HB2	4:B:77:LYS:HE2	1.86	0.43
4:A:73:ARG:NH1	4:A:103:LYS:HD2	2.33	0.43
4:B:235:GLN:OE1	4:B:235:GLN:N	2.43	0.43
4:A:129:SER:OG	4:A:130:GLY:N	2.51	0.42
4:B:265:THR:HG23	4:B:281:ARG:HG3	2.00	0.42
4:B:114:LEU:HB3	4:B:134:LEU:HB3	2.02	0.42
4:B:177:ARG:O	4:B:180:VAL:HG13	2.19	0.42
4:A:73:ARG:O	4:A:77:LYS:HG3	2.19	0.42
1:C:9:DT:H2''	1:C:10:DC:C6	2.54	0.42
3:E:19:DA:H2'	9:E:102:HOH:O	2.20	0.42
4:B:95:GLN:HA	4:B:131:VAL:HG12	2.02	0.42
4:A:179:LEU:HD13	4:A:182:LEU:HD22	2.00	0.42
4:A:227:LYS:HD2	4:A:227:LYS:HA	1.66	0.41
4:B:285:PHE:CD2	4:B:314:LEU:HB2	2.56	0.41
1:C:7:DG:H2''	1:C:8:DA:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:95:GLN:HB3	4:B:171:TYR:HB2	2.02	0.41
4:B:81:LEU:HA	4:B:81:LEU:HD23	1.88	0.41
4:A:318:LEU:HD23	4:A:318:LEU:HA	1.72	0.41
3:E:19:DA:H8	9:E:102:HOH:O	2.03	0.41
4:B:202:ARG:HD2	6:B:401:EDO:C2	2.51	0.41
4:A:109:GLN:OE1	4:A:109:GLN:HA	2.20	0.41
4:B:92:LEU:HD21	4:B:94:LEU:HD21	2.02	0.41
1:C:4:DA:N6	3:E:7:DG:H1	2.18	0.40
4:A:111:LEU:HA	4:A:111:LEU:HD23	1.82	0.40
4:B:194:LYS:HD2	4:B:194:LYS:HA	1.72	0.40
2:D:10[A]:C7R:C6	4:B:280:TRP:CZ2	3.04	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	275/276 (100%)	262 (95%)	13 (5%)	0	100	100
4	B	275/276 (100%)	268 (98%)	7 (2%)	0	100	100
All	All	550/552 (100%)	530 (96%)	20 (4%)	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	
4	A	234/236 (99%)	234 (100%)	0	100	100
4	B	234/236 (99%)	233 (100%)	1 (0%)	91	96
All	All	468/472 (99%)	467 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	203	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C7S	D	10[B]	2	15,20,21	5.38	12 (80%)	17,28,31	2.16	5 (29%)
2	C7R	D	10[A]	2	15,20,21	5.53	12 (80%)	17,28,31	2.14	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C7S	D	10[B]	2	-	2/3/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C7R	D	10[A]	2	-	3/3/21/22	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10[A]	C7R	C2'-C3'	-11.53	1.22	1.52
2	D	10[B]	C7S	C2'-C3'	-11.46	1.22	1.52
2	D	10[B]	C7S	O4'-C4'	-8.51	1.26	1.45
2	D	10[A]	C7R	O4'-C4'	-8.27	1.26	1.45
2	D	10[A]	C7R	C6-N1	7.75	1.45	1.35
2	D	10[B]	C7S	C6-N1	7.30	1.44	1.35
2	D	10[A]	C7R	C4-N3	6.04	1.45	1.35
2	D	10[A]	C7R	C2-N3	5.49	1.49	1.38
2	D	10[A]	C7R	C6-C5	5.39	1.50	1.38
2	D	10[B]	C7S	C4-N3	5.37	1.44	1.35
2	D	10[B]	C7S	C6-C5	5.25	1.49	1.38
2	D	10[A]	C7R	C1'-N1	-5.22	1.33	1.49
2	D	10[B]	C7S	C2-N3	5.22	1.48	1.38
2	D	10[B]	C7S	C3'-C4'	5.12	1.67	1.53
2	D	10[A]	C7R	C3'-C4'	4.81	1.66	1.53
2	D	10[B]	C7S	C1'-N1	-4.62	1.35	1.49
2	D	10[A]	C7R	C4-N4	3.58	1.45	1.35
2	D	10[A]	C7R	C5-C4	3.40	1.49	1.41
2	D	10[B]	C7S	O3'-C3'	3.33	1.50	1.43
2	D	10[B]	C7S	O4'-C1'	3.26	1.49	1.42
2	D	10[A]	C7R	O4'-C1'	3.24	1.49	1.42
2	D	10[A]	C7R	O3'-C3'	3.23	1.50	1.43
2	D	10[B]	C7S	C4-N4	3.17	1.44	1.35
2	D	10[B]	C7S	C5-C4	3.05	1.48	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10[A]	C7R	C4'-O4'-C1'	-6.42	93.95	109.45
2	D	10[B]	C7S	C4'-O4'-C1'	-4.45	98.71	109.45
2	D	10[B]	C7S	O4'-C1'-C2'	-3.92	98.85	106.25
2	D	10[A]	C7R	C2-N3-C4	3.80	120.19	116.34
2	D	10[B]	C7S	O5'-C5'-C4'	3.29	120.17	108.99
2	D	10[B]	C7S	C2-N3-C4	3.07	119.45	116.34
2	D	10[B]	C7S	N4-C4-N3	2.64	120.66	116.49
2	D	10[A]	C7R	N4-C4-N3	2.31	120.14	116.49
2	D	10[A]	C7R	C2'-C1'-N1	-2.22	109.14	114.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	10[B]	C7S	O4'-C4'-C5'-O5'
2	D	10[A]	C7R	O4'-C1'-N1-C6
2	D	10[B]	C7S	C3'-C4'-C5'-O5'
2	D	10[A]	C7R	O4'-C4'-C5'-O5'
2	D	10[A]	C7R	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	10[A]	C7R	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	EDO	A	401	-	3,3,3	0.55	0	2,2,2	0.20	0
6	EDO	B	401	-	3,3,3	0.32	0	2,2,2	0.58	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	EDO	A	401	-	-	0/1/1/1	-
6	EDO	B	401	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	401	EDO	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 [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	C	11/11 (100%)	0.53	1 (9%) 9 8	66, 100, 114, 115	0
2	D	9/11 (81%)	-0.32	0 100 100	47, 52, 56, 59	0
3	E	21/21 (100%)	0.36	2 (9%) 8 7	49, 66, 110, 116	0
4	A	276/276 (100%)	-0.20	0 100 100	35, 46, 63, 79	0
4	B	276/276 (100%)	-0.21	1 (0%) 92 91	32, 43, 60, 74	0
All	All	593/595 (99%)	-0.17	4 (0%) 87 86	32, 45, 68, 116	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1	DG	2.9
1	C	11	DC	2.6
3	E	12	DT	2.5
4	B	112	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	C7S	D	10[B]	19/20	0.65	0.47	60,66,71,76	19
2	C7R	D	10[A]	19/20	0.74	0.55	59,64,67,75	19

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

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(Å <sup>2</sup> )	Q<0.9
5	CA	D	101	1/1	0.86	0.09	79,79,79,79	0
8	CL	A	403	1/1	0.88	0.09	83,83,83,83	0
6	EDO	B	401	4/4	0.89	0.23	56,58,61,61	0
6	EDO	A	401	4/4	0.94	0.27	54,56,60,61	0
7	NA	A	402	1/1	0.98	0.14	45,45,45,45	0

## 6.5 Other polymers

There are no such residues in this entry.