



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 AM GMT

PDB ID : 3CDU  
Title : Crystal structure of coxsackievirus B3 RNA-dependent RNA polymerase (3Dpol) in complex with a pyrophosphate  
Authors : Gruez, A.; Selisko, B.; Roberts, M.; Bricogne, G.; Bussetta, C.; Canard, B.  
Deposited on : 2008-02-27  
Resolution : 2.10 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  
<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

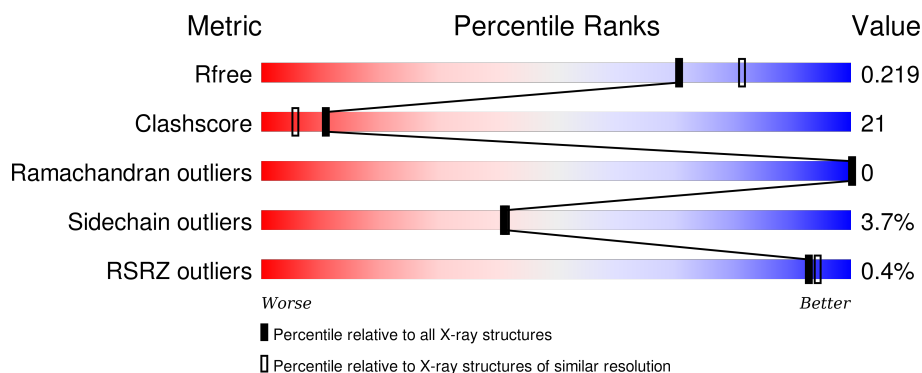
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	468	

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
3	SO4	A	475	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	477	-	-	X	-
4	ACT	A	478	-	-	X	X
4	ACT	A	480	-	-	-	X
5	POP	A	482	-	-	X	X
6	GOL	A	484	-	-	-	X
6	GOL	A	485	-	-	-	X
6	GOL	A	487	-	-	X	-
6	GOL	A	489	-	-	X	X
6	GOL	A	490	-	-	-	X
6	GOL	A	491	-	-	-	X
6	GOL	A	492	-	-	X	X
6	GOL	A	493	-	-	-	X
6	GOL	A	494	-	-	-	X
6	GOL	A	495	-	-	-	X
6	GOL	A	496	-	-	-	X
6	GOL	A	497	-	-	-	X
6	GOL	A	498	-	-	X	X
6	GOL	A	499	-	-	-	X
6	GOL	A	500	-	-	X	X
6	GOL	A	501	-	-	X	X
6	GOL	A	502	-	-	X	X
6	GOL	A	504	-	-	-	X
6	GOL	A	505	-	-	X	X
6	GOL	A	506	-	-	X	X
6	GOL	A	507	-	-	-	X
6	GOL	A	509	-	-	-	X
6	GOL	A	510	-	-	-	X
6	GOL	A	511	-	-	X	-
6	GOL	A	512	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4323 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 RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	6	0
			3778	2420	641	695	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	HIS	-	EXPRESSION TAG	UNP P03313
A	464	HIS	-	EXPRESSION TAG	UNP P03313
A	465	HIS	-	EXPRESSION TAG	UNP P03313
A	466	HIS	-	EXPRESSION TAG	UNP P03313
A	467	HIS	-	EXPRESSION TAG	UNP P03313
A	468	HIS	-	EXPRESSION TAG	UNP P03313

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cl	0	0
			6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



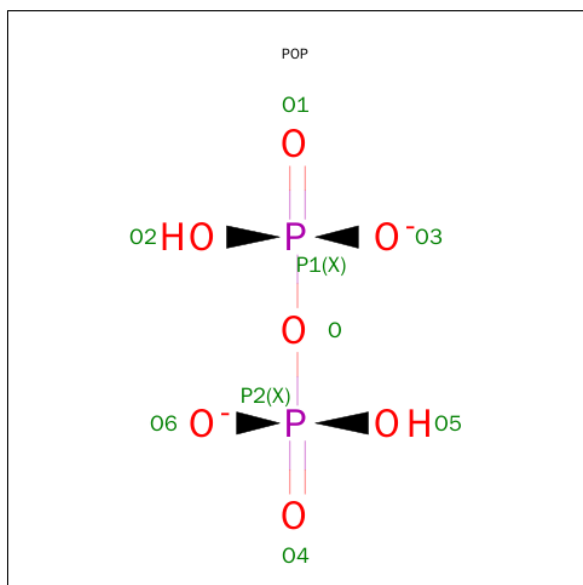
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

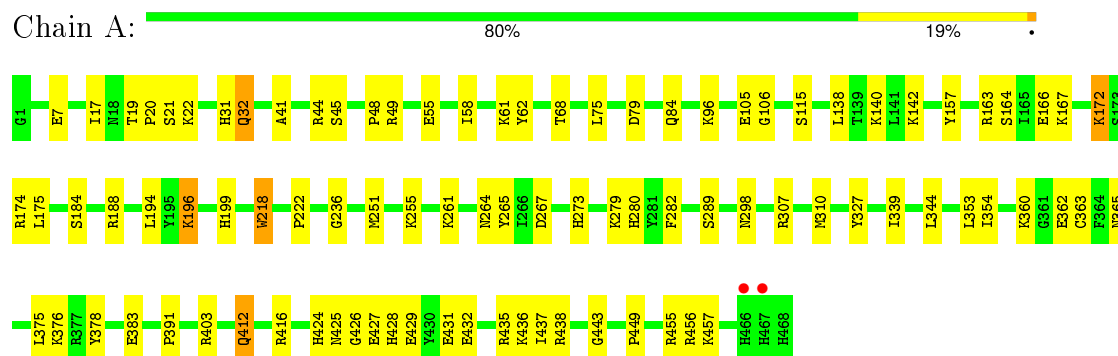
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	321	Total O 321 321	0	0



### 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 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: RNA-directed RNA polymerase 3D-POL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.41Å 74.41Å 285.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.98 – 2.10 72.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.7 (71.98-2.10) 84.8 (72.01-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.95 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT 2.3.0	Depositor
R, $R_{free}$	0.178 , 0.220 0.175 , 0.219	Depositor DCC
$R_{free}$ test set	2045 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40824 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4323	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, 0.375 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: GOL, ACT, SO4, POP, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	0/3905	0.71	0/5284

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

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	3778	0	3723	151	0
2	A	6	0	0	0	0
3	A	5	0	0	0	0
4	A	24	0	18	21	0
5	A	9	0	0	6	0
6	A	180	0	239	91	0
7	A	321	0	0	12	0
All	All	4323	0	3980	168	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 21.

All (168) 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)
1:A:273[A]:HIS:NE2	1:A:280:HIS:NE2	2.03	1.05
1:A:61:LYS:HD2	6:A:500:GOL:H11	1.39	1.04
1:A:360:LYS:NZ	6:A:492:GOL:H32	1.84	0.93
1:A:61:LYS:HD2	6:A:500:GOL:C1	2.00	0.91
1:A:310:MET:HE1	1:A:339:ILE:HG21	1.51	0.90
1:A:61:LYS:NZ	6:A:500:GOL:H12	1.88	0.88
1:A:455:ARG:HH21	6:A:486:GOL:H12	1.37	0.88
1:A:403:ARG:HH22	6:A:505:GOL:H12	1.40	0.85
1:A:31:HIS:CE1	6:A:505:GOL:H31	2.11	0.85
1:A:403:ARG:NH2	6:A:505:GOL:H12	1.97	0.79
1:A:424:HIS:O	6:A:499:GOL:H12	1.80	0.79
1:A:427:GLU:O	1:A:431[A]:GLU:HG3	1.82	0.78
1:A:429:GLU:HG2	4:A:478:ACT:H2	1.65	0.78
1:A:383:GLU:HB2	6:A:506:GOL:H12	1.66	0.76
1:A:49:ARG:HG3	6:A:511:GOL:H11	1.66	0.76
1:A:45:SER:H	6:A:498:GOL:C3	1.99	0.76
1:A:31:HIS:NE2	6:A:505:GOL:H31	1.99	0.75
1:A:279:LYS:HG3	6:A:497:GOL:H12	1.68	0.75
1:A:167[B]:LYS:NZ	5:A:482:POP:O6	2.21	0.74
1:A:264:ASN:HB3	6:A:495:GOL:H31	1.69	0.74
1:A:429:GLU:HG2	4:A:478:ACT:C	2.19	0.73
1:A:17:ILE:HG22	1:A:19:THR:HG23	1.68	0.73
1:A:172:LYS:HE2	1:A:172:LYS:HA	1.72	0.72
6:A:499:GOL:H31	6:A:506:GOL:O2	1.90	0.71
1:A:49:ARG:HD3	6:A:511:GOL:O1	1.91	0.71
1:A:438:ARG:NH1	7:A:813:HOH:O	2.24	0.71
1:A:49:ARG:CG	6:A:511:GOL:H11	2.21	0.70
1:A:163[B]:ARG:NH2	5:A:482:POP:O1	2.24	0.70
1:A:383:GLU:CB	6:A:506:GOL:H12	2.20	0.70
1:A:61:LYS:HZ2	6:A:500:GOL:H12	1.54	0.70
1:A:429:GLU:HG2	4:A:478:ACT:CH3	2.22	0.69
6:A:489:GOL:H11	7:A:751:HOH:O	1.93	0.68
1:A:45:SER:OG	6:A:498:GOL:H32	1.92	0.68
1:A:22:LYS:CE	4:A:477:ACT:H3	2.26	0.66
6:A:489:GOL:H32	7:A:751:HOH:O	1.95	0.65
1:A:360:LYS:HZ1	6:A:492:GOL:H32	1.60	0.65
1:A:172:LYS:CA	1:A:172:LYS:HE2	2.23	0.65
6:A:484:GOL:H2	6:A:504:GOL:O2	1.98	0.64
1:A:184:SER:O	1:A:188:ARG:HG3	1.98	0.64
6:A:493:GOL:H12	7:A:673:HOH:O	1.97	0.64
1:A:49:ARG:HE	6:A:511:GOL:H32	1.64	0.63
1:A:273[B]:HIS:HB3	1:A:282:PHE:CE1	2.33	0.63

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HB2	1:A:163[B]:ARG:HG3	1.79	0.63
1:A:84:GLN:NE2	1:A:307:ARG:HH21	1.96	0.62
1:A:412:GLN:NE2	7:A:658:HOH:O	2.31	0.62
1:A:49:ARG:NE	6:A:511:GOL:H32	2.15	0.61
1:A:416:ARG:HD3	7:A:758:HOH:O	1.99	0.61
1:A:19:THR:HB	1:A:20:PRO:HD2	1.83	0.61
1:A:172:LYS:CE	1:A:172:LYS:HA	2.31	0.60
1:A:44:ARG:HH21	4:A:477:ACT:C	2.15	0.60
1:A:61:LYS:HZ3	6:A:500:GOL:H12	1.66	0.60
1:A:383:GLU:HB2	6:A:506:GOL:C1	2.31	0.60
1:A:45:SER:H	6:A:498:GOL:H32	1.67	0.60
6:A:484:GOL:H12	7:A:629:HOH:O	2.02	0.60
1:A:360:LYS:HZ3	6:A:492:GOL:H32	1.67	0.60
1:A:115:SER:N	6:A:510:GOL:O1	2.29	0.60
1:A:45:SER:H	6:A:498:GOL:H31	1.67	0.60
1:A:310:MET:HE3	1:A:344:LEU:HD21	1.84	0.59
1:A:61:LYS:HB2	6:A:501:GOL:O1	2.02	0.59
1:A:426:GLY:HA3	4:A:478:ACT:O	2.03	0.58
1:A:22:LYS:HE2	4:A:477:ACT:H3	1.86	0.58
1:A:273[A]:HIS:CD2	1:A:280:HIS:NE2	2.70	0.58
1:A:456:ARG:NE	6:A:487:GOL:O1	2.33	0.58
1:A:360:LYS:CE	6:A:492:GOL:H32	2.34	0.58
1:A:425:ASN:O	4:A:478:ACT:O	2.22	0.58
6:A:505:GOL:H32	7:A:560:HOH:O	2.05	0.57
1:A:19:THR:HG22	1:A:157:TYR:CE1	2.40	0.57
1:A:427:GLU:H	6:A:507:GOL:H2	1.69	0.57
1:A:61:LYS:HD2	6:A:500:GOL:H12	1.87	0.56
6:A:499:GOL:H31	6:A:506:GOL:O1	2.06	0.56
1:A:44:ARG:NH2	4:A:477:ACT:O	2.38	0.56
1:A:264:ASN:CB	6:A:495:GOL:H31	2.35	0.56
1:A:44:ARG:HA	6:A:498:GOL:H31	1.89	0.55
1:A:267:ASP:OD1	6:A:496:GOL:H12	2.06	0.55
4:A:480:ACT:H2	6:A:496:GOL:O3	2.06	0.55
1:A:138:LEU:O	1:A:142:LYS:HG3	2.06	0.55
1:A:429:GLU:N	4:A:478:ACT:OXT	2.38	0.55
1:A:378:TYR:CD2	6:A:490:GOL:H12	2.42	0.54
5:A:482:POP:O6	5:A:482:POP:O1	2.26	0.53
1:A:105:GLU:O	1:A:196:LYS:HD2	2.09	0.53
1:A:84:GLN:HE22	1:A:307:ARG:NH2	2.06	0.53
6:A:502:GOL:H32	7:A:650:HOH:O	2.09	0.52
1:A:360:LYS:HE2	6:A:492:GOL:C3	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HE22	1:A:307:ARG:HH21	1.58	0.52
1:A:456:ARG:HE	6:A:487:GOL:HO1	1.56	0.52
1:A:7:GLU:OE2	1:A:280:HIS:ND1	2.32	0.51
6:A:487:GOL:O1	6:A:487:GOL:O3	2.28	0.51
1:A:164:SER:N	5:A:482:POP:O5	2.34	0.51
1:A:279:LYS:HG3	6:A:497:GOL:C1	2.38	0.51
1:A:403:ARG:HH22	6:A:505:GOL:C1	2.19	0.51
1:A:22:LYS:HD2	4:A:477:ACT:H2	1.93	0.51
1:A:106:GLY:O	1:A:199:HIS:HD2	1.92	0.51
1:A:435:ARG:HG2	1:A:435:ARG:HH11	1.76	0.51
1:A:429:GLU:CG	4:A:478:ACT:H2	2.38	0.51
1:A:44:ARG:NE	4:A:477:ACT:O	2.42	0.51
1:A:416:ARG:HH22	6:A:489:GOL:C1	2.24	0.51
1:A:115:SER:H	6:A:510:GOL:H32	1.76	0.51
1:A:236:GLY:H	6:A:502:GOL:C1	2.24	0.50
1:A:457:LYS:HE3	6:A:488:GOL:H11	1.92	0.50
1:A:21:SER:N	4:A:476:ACT:OXT	2.29	0.50
1:A:429:GLU:H	4:A:478:ACT:C	2.22	0.50
1:A:383:GLU:CG	6:A:506:GOL:H12	2.42	0.49
1:A:84:GLN:NE2	1:A:307:ARG:NH2	2.61	0.49
1:A:363:CYS:O	1:A:365:ASN:N	2.46	0.49
1:A:353:LEU:C	1:A:354:ILE:HD13	2.33	0.49
1:A:218:TRP:CD1	1:A:391:PRO:HA	2.47	0.49
1:A:236:GLY:H	6:A:502:GOL:H12	1.79	0.48
1:A:174[A]:ARG:NH1	6:A:502:GOL:C3	2.75	0.48
1:A:62:TYR:CZ	6:A:501:GOL:H32	2.49	0.48
1:A:194:LEU:C	1:A:194:LEU:HD23	2.34	0.48
1:A:19:THR:CG2	1:A:157:TYR:CE1	2.96	0.48
1:A:429:GLU:CG	4:A:478:ACT:C	2.89	0.48
1:A:435:ARG:HG2	1:A:435:ARG:NH1	2.29	0.48
1:A:62:TYR:CD2	6:A:501:GOL:H12	2.49	0.47
6:A:511:GOL:O1	6:A:512:GOL:H32	2.14	0.47
1:A:79:ASP:OD1	1:A:255:LYS:HE2	2.15	0.47
1:A:174[A]:ARG:NH2	5:A:482:POP:O1	2.45	0.47
1:A:49:ARG:HD3	6:A:511:GOL:C1	2.44	0.47
1:A:75:LEU:HD23	1:A:251:MET:HE1	1.97	0.47
1:A:428:HIS:N	4:A:478:ACT:OXT	2.48	0.47
1:A:45:SER:CB	6:A:498:GOL:H32	2.45	0.47
1:A:375:LEU:O	1:A:376:LYS:HB2	2.15	0.47
1:A:48:PRO:HG2	6:A:511:GOL:H2	1.97	0.46
1:A:174[A]:ARG:NH1	6:A:502:GOL:H31	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HE1	1:A:339:ILE:CG2	2.36	0.46
1:A:19:THR:HG21	1:A:157:TYR:CD1	2.51	0.46
1:A:432:GLU:HG3	1:A:436:LYS:HE2	1.97	0.46
1:A:222:PRO:HG2	6:A:491:GOL:H11	1.98	0.46
1:A:251:MET:HE3	1:A:251:MET:HB3	1.80	0.46
1:A:22:LYS:HD2	4:A:477:ACT:CH3	2.46	0.46
1:A:437:ILE:O	1:A:443:GLY:HA3	2.17	0.45
1:A:163[A]:ARG:NH1	1:A:174[A]:ARG:HG3	2.32	0.45
1:A:164:SER:HG	6:A:492:GOL:HO2	1.64	0.45
1:A:62:TYR:CZ	6:A:501:GOL:C3	3.01	0.44
1:A:383:GLU:H	6:A:506:GOL:C1	2.31	0.44
1:A:75:LEU:CD2	1:A:251:MET:HE1	2.47	0.44
1:A:172:LYS:CE	1:A:172:LYS:CA	2.94	0.44
1:A:167[B]:LYS:HE3	6:A:492:GOL:O3	2.18	0.44
1:A:164:SER:OG	6:A:492:GOL:O2	2.31	0.44
6:A:483:GOL:H31	6:A:484:GOL:H31	2.00	0.44
1:A:455:ARG:NH2	6:A:486:GOL:H12	2.18	0.44
1:A:174[A]:ARG:HH12	6:A:502:GOL:H31	1.81	0.43
1:A:17:ILE:CG2	1:A:19:THR:HG23	2.42	0.43
1:A:383:GLU:H	6:A:506:GOL:H12	1.83	0.43
1:A:456:ARG:NH2	6:A:487:GOL:O1	2.47	0.43
1:A:164:SER:OG	1:A:167[A]:LYS:HG2	2.18	0.43
1:A:438:ARG:NH2	7:A:759:HOH:O	2.47	0.43
5:A:482:POP:O4	6:A:492:GOL:O3	2.29	0.43
1:A:174[A]:ARG:NH1	6:A:502:GOL:O3	2.46	0.43
1:A:428:HIS:HB3	4:A:478:ACT:OXT	2.18	0.43
1:A:22:LYS:CD	4:A:477:ACT:CH3	2.97	0.43
1:A:45:SER:N	6:A:498:GOL:H31	2.31	0.43
1:A:61:LYS:HB2	6:A:501:GOL:C1	2.49	0.42
1:A:32:GLN:HB2	7:A:523:HOH:O	2.19	0.42
1:A:58:ILE:HD12	1:A:175:LEU:HD21	2.01	0.42
1:A:456:ARG:HH22	6:A:488:GOL:C1	2.33	0.42
1:A:360:LYS:HE2	6:A:492:GOL:C2	2.49	0.42
1:A:383:GLU:HB2	6:A:506:GOL:C2	2.50	0.41
1:A:438:ARG:NE	7:A:759:HOH:O	2.27	0.41
1:A:61:LYS:CD	6:A:500:GOL:C1	2.87	0.41
1:A:106:GLY:O	1:A:199:HIS:CD2	2.73	0.41
1:A:164:SER:OG	1:A:167[B]:LYS:HG3	2.20	0.41
1:A:449:PRO:HA	6:A:489:GOL:H12	2.01	0.41
1:A:427:GLU:N	6:A:507:GOL:H2	2.35	0.41
1:A:218:TRP:O	1:A:222:PRO:HD3	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	6:A:498:GOL:O3	2.36	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
1	A	472/468 (101%)	465 (98%)	7 (2%)	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	415/409 (102%)	400 (96%)	15 (4%)	42 43

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	68	THR
1	A	96	LYS
1	A	140	LYS
1	A	166	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	172	LYS
1	A	196	LYS
1	A	218	TRP
1	A	261	LYS
1	A	265	TYR
1	A	289	SER
1	A	298	ASN
1	A	327	TYR
1	A	362	GLU
1	A	412	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	199	HIS
1	A	228	HIS
1	A	271	ASN
1	A	298	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 6 are monoatomic - leaving 38 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	$\# Z  > 2$
3	SO4	A	475	-	4,4,4	0.88	0	6,6,6	0.18	0
4	ACT	A	476	-	1,3,3	3.06	1 (100%)	0,3,3	0.00	-
4	ACT	A	477	-	1,3,3	3.63	1 (100%)	0,3,3	0.00	-
4	ACT	A	478	-	1,3,3	3.70	1 (100%)	0,3,3	0.00	-
4	ACT	A	479	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
4	ACT	A	480	-	1,3,3	2.33	1 (100%)	0,3,3	0.00	-
4	ACT	A	481	-	1,3,3	2.96	1 (100%)	0,3,3	0.00	-
5	POP	A	482	-	8,8,8	2.23	3 (37%)	13,13,13	3.14	5 (38%)
6	GOL	A	483	-	5,5,5	0.72	0	5,5,5	1.46	1 (20%)
6	GOL	A	484	-	5,5,5	1.16	0	5,5,5	1.18	0
6	GOL	A	485	-	5,5,5	0.37	0	5,5,5	1.13	0
6	GOL	A	486	-	5,5,5	0.61	0	5,5,5	1.00	0
6	GOL	A	487	-	5,5,5	0.18	0	5,5,5	0.54	0
6	GOL	A	488	-	5,5,5	0.52	0	5,5,5	0.54	0
6	GOL	A	489	-	5,5,5	0.89	0	5,5,5	1.46	1 (20%)
6	GOL	A	490	-	5,5,5	0.30	0	5,5,5	1.05	0
6	GOL	A	491	-	5,5,5	0.83	0	5,5,5	1.84	2 (40%)
6	GOL	A	492	-	5,5,5	0.81	0	5,5,5	0.51	0
6	GOL	A	493	-	5,5,5	0.76	0	5,5,5	0.92	0
6	GOL	A	494	-	5,5,5	0.57	0	5,5,5	1.28	0
6	GOL	A	495	-	5,5,5	0.49	0	5,5,5	1.07	0
6	GOL	A	496	-	5,5,5	0.32	0	5,5,5	0.82	0
6	GOL	A	497	-	5,5,5	0.61	0	5,5,5	0.72	0
6	GOL	A	498	-	5,5,5	0.93	0	5,5,5	1.45	1 (20%)
6	GOL	A	499	-	5,5,5	0.76	0	5,5,5	0.91	0
6	GOL	A	500	-	5,5,5	1.38	0	5,5,5	1.38	1 (20%)
6	GOL	A	501	-	5,5,5	1.73	2 (40%)	5,5,5	1.27	1 (20%)
6	GOL	A	502	-	5,5,5	0.78	0	5,5,5	0.58	0
6	GOL	A	503	-	5,5,5	0.48	0	5,5,5	0.47	0
6	GOL	A	504	-	5,5,5	0.49	0	5,5,5	1.49	1 (20%)
6	GOL	A	505	-	5,5,5	0.73	0	5,5,5	0.76	0
6	GOL	A	506	-	5,5,5	0.63	0	5,5,5	1.56	1 (20%)
6	GOL	A	507	-	5,5,5	0.79	0	5,5,5	1.02	0
6	GOL	A	508	-	5,5,5	1.09	0	5,5,5	1.25	0
6	GOL	A	509	-	5,5,5	0.64	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	510	-	5,5,5	0.84	0	5,5,5	2.54	2 (40%)
6	GOL	A	511	-	5,5,5	0.78	0	5,5,5	1.00	0
6	GOL	A	512	-	5,5,5	0.58	0	5,5,5	0.45	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
3	SO4	A	475	-	-	0/0/0/0	0/0/0/0
4	ACT	A	476	-	-	0/0/0/0	0/0/0/0
4	ACT	A	477	-	-	0/0/0/0	0/0/0/0
4	ACT	A	478	-	-	0/0/0/0	0/0/0/0
4	ACT	A	479	-	-	0/0/0/0	0/0/0/0
4	ACT	A	480	-	-	0/0/0/0	0/0/0/0
4	ACT	A	481	-	-	0/0/0/0	0/0/0/0
5	POP	A	482	-	-	0/6/6/6	0/0/0/0
6	GOL	A	483	-	-	0/4/4/4	0/0/0/0
6	GOL	A	484	-	-	0/4/4/4	0/0/0/0
6	GOL	A	485	-	-	0/4/4/4	0/0/0/0
6	GOL	A	486	-	-	0/4/4/4	0/0/0/0
6	GOL	A	487	-	-	0/4/4/4	0/0/0/0
6	GOL	A	488	-	-	0/4/4/4	0/0/0/0
6	GOL	A	489	-	-	0/4/4/4	0/0/0/0
6	GOL	A	490	-	-	0/4/4/4	0/0/0/0
6	GOL	A	491	-	-	0/4/4/4	0/0/0/0
6	GOL	A	492	-	-	0/4/4/4	0/0/0/0
6	GOL	A	493	-	-	0/4/4/4	0/0/0/0
6	GOL	A	494	-	-	0/4/4/4	0/0/0/0
6	GOL	A	495	-	-	0/4/4/4	0/0/0/0
6	GOL	A	496	-	-	0/4/4/4	0/0/0/0
6	GOL	A	497	-	-	0/4/4/4	0/0/0/0
6	GOL	A	498	-	-	0/4/4/4	0/0/0/0
6	GOL	A	499	-	-	0/4/4/4	0/0/0/0
6	GOL	A	500	-	-	0/4/4/4	0/0/0/0
6	GOL	A	501	-	-	0/4/4/4	0/0/0/0
6	GOL	A	502	-	-	0/4/4/4	0/0/0/0
6	GOL	A	503	-	-	0/4/4/4	0/0/0/0
6	GOL	A	504	-	-	0/4/4/4	0/0/0/0
6	GOL	A	505	-	-	0/4/4/4	0/0/0/0
6	GOL	A	506	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	507	-	-	0/4/4/4	0/0/0/0
6	GOL	A	508	-	-	0/4/4/4	0/0/0/0
6	GOL	A	509	-	-	0/4/4/4	0/0/0/0
6	GOL	A	510	-	-	0/4/4/4	0/0/0/0
6	GOL	A	511	-	-	0/4/4/4	0/0/0/0
6	GOL	A	512	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	GOL	O2-C2	-2.62	1.35	1.43
6	A	501	GOL	C1-C2	2.04	1.60	1.52
4	A	480	ACT	CH3-C	2.33	1.52	1.48
4	A	481	ACT	CH3-C	2.96	1.52	1.48
5	A	482	POP	P2-O	2.99	1.67	1.61
4	A	476	ACT	CH3-C	3.06	1.53	1.48
5	A	482	POP	P2-O4	3.22	1.60	1.50
5	A	482	POP	P1-O	3.33	1.68	1.61
4	A	479	ACT	CH3-C	3.41	1.53	1.48
4	A	477	ACT	CH3-C	3.63	1.53	1.48
4	A	478	ACT	CH3-C	3.70	1.53	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	482	POP	P2-O-P1	-8.42	109.09	132.73
5	A	482	POP	O3-P1-O1	-4.29	94.10	114.72
5	A	482	POP	O6-P2-O4	-4.24	94.35	114.72
6	A	510	GOL	C3-C2-C1	-3.75	96.40	111.12
6	A	510	GOL	O1-C1-C2	-3.51	93.17	110.18
6	A	491	GOL	C3-C2-C1	-2.81	100.11	111.12
6	A	504	GOL	O3-C3-C2	-2.64	97.40	110.18
6	A	491	GOL	O3-C3-C2	-2.49	98.12	110.18
6	A	506	GOL	O1-C1-C2	-2.43	98.38	110.18
6	A	489	GOL	O2-C2-C1	-2.36	97.85	108.65
6	A	501	GOL	O2-C2-C3	-2.01	99.42	108.65
5	A	482	POP	O2-P1-O	2.01	113.87	104.65
6	A	500	GOL	O2-C2-C3	2.06	118.08	108.65
6	A	498	GOL	O1-C1-C2	2.10	120.38	110.18
6	A	483	GOL	C3-C2-C1	2.41	120.58	111.12
5	A	482	POP	O5-P2-O	2.92	118.07	104.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	476	ACT	1	0
4	A	477	ACT	8	0
4	A	478	ACT	11	0
4	A	480	ACT	1	0
5	A	482	POP	6	0
6	A	483	GOL	1	0
6	A	484	GOL	3	0
6	A	486	GOL	2	0
6	A	487	GOL	4	0
6	A	488	GOL	2	0
6	A	489	GOL	4	0
6	A	490	GOL	1	0
6	A	491	GOL	1	0
6	A	492	GOL	10	0
6	A	493	GOL	1	0
6	A	495	GOL	2	0
6	A	496	GOL	2	0
6	A	497	GOL	2	0
6	A	498	GOL	8	0
6	A	499	GOL	3	0
6	A	500	GOL	9	0
6	A	501	GOL	5	0
6	A	502	GOL	7	0
6	A	504	GOL	1	0
6	A	505	GOL	6	0
6	A	506	GOL	9	0
6	A	507	GOL	2	0
6	A	510	GOL	2	0
6	A	511	GOL	8	0
6	A	512	GOL	1	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	A	468/468 (100%)	-0.35	2 (0%) 93 94	16, 26, 50, 75	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	HIS	4.9
1	A	466	HIS	3.1

### 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	512	6/6	0.59	0.41	45.22	84,85,85,87	0
6	GOL	A	506	6/6	0.87	0.43	31.00	57,61,62,64	0
6	GOL	A	484	6/6	0.64	0.33	21.36	60,63,63,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACT	A	478	4/4	0.83	0.43	20.55	65,65,65,66	0
6	GOL	A	494	6/6	0.93	0.25	16.56	54,57,58,59	0
6	GOL	A	500	6/6	0.80	0.41	13.21	36,40,41,42	0
6	GOL	A	499	6/6	0.86	0.23	12.44	45,47,47,49	0
6	GOL	A	493	6/6	0.91	0.20	11.76	39,47,48,51	0
6	GOL	A	507	6/6	0.80	0.29	11.22	51,54,54,57	0
6	GOL	A	490	6/6	0.94	0.20	9.64	58,61,62,63	0
6	GOL	A	505	6/6	0.72	0.23	9.40	58,61,62,63	0
6	GOL	A	504	6/6	0.94	0.19	8.80	38,38,39,42	0
6	GOL	A	497	6/6	0.80	0.27	8.15	58,60,61,63	0
6	GOL	A	491	6/6	0.94	0.18	8.05	47,49,50,52	0
6	GOL	A	510	6/6	0.89	0.28	6.98	53,55,55,57	0
6	GOL	A	496	6/6	0.91	0.18	6.80	54,56,56,58	0
5	POP	A	482	9/9	0.86	0.24	6.52	35,36,39,39	9
6	GOL	A	498	6/6	0.78	0.30	5.88	63,63,64,65	0
6	GOL	A	509	6/6	0.80	0.21	5.58	65,67,67,68	0
6	GOL	A	502	6/6	0.76	0.27	5.57	63,68,69,69	0
6	GOL	A	501	6/6	0.92	0.23	5.27	42,43,43,44	0
6	GOL	A	489	6/6	0.88	0.20	5.06	45,48,48,50	0
6	GOL	A	495	6/6	0.91	0.17	4.56	63,64,65,66	0
3	SO4	A	475	5/5	0.90	0.18	4.41	82,85,86,87	0
6	GOL	A	485	6/6	0.94	0.17	3.23	30,37,39,43	0
4	ACT	A	480	4/4	0.84	0.28	3.20	72,72,73,73	0
6	GOL	A	492	6/6	0.86	0.28	2.66	56,57,58,58	0
6	GOL	A	503	6/6	0.98	0.09	0.55	30,32,34,37	0
2	CL	A	469	1/1	0.99	0.10	0.10	30,30,30,30	0
2	CL	A	470	1/1	0.99	0.09	-0.92	31,31,31,31	0
2	CL	A	472	1/1	1.00	0.05	-2.18	30,30,30,30	0
2	CL	A	474	1/1	0.87	0.09	-2.92	91,91,91,91	0
6	GOL	A	486	6/6	0.87	0.13	-	51,51,51,53	0
4	ACT	A	481	4/4	0.87	0.17	-	70,70,70,71	0
4	ACT	A	479	4/4	0.33	0.35	-	89,90,91,91	0
2	CL	A	471	1/1	1.00	0.07	-	34,34,34,34	0
6	GOL	A	508	6/6	0.62	0.30	-	63,65,65,66	0
4	ACT	A	477	4/4	0.69	0.42	-	60,61,61,61	0
2	CL	A	473	1/1	0.97	0.08	-	48,48,48,48	0
6	GOL	A	487	6/6	0.91	0.29	-	64,64,65,66	0
4	ACT	A	476	4/4	0.79	0.17	-	63,64,64,65	0
6	GOL	A	483	6/6	0.87	0.27	-	40,44,45,49	0
6	GOL	A	488	6/6	0.89	0.23	-	82,83,84,84	0
6	GOL	A	511	6/6	0.80	0.68	-	52,58,60,61	0



## 6.5 Other polymers

There are no such residues in this entry.