



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:00 am GMT

PDB ID : 3WXL  
Title : Crystal structure of trypanosoma brucei gambiense glycerol kinase complex with adp, mg2+, and glycerol  
Authors : Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Kido, Y.; Tsuge, C.; Nara, T.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Kita, K.; Harada, S.  
Deposited on : 2014-08-01  
Resolution : 1.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

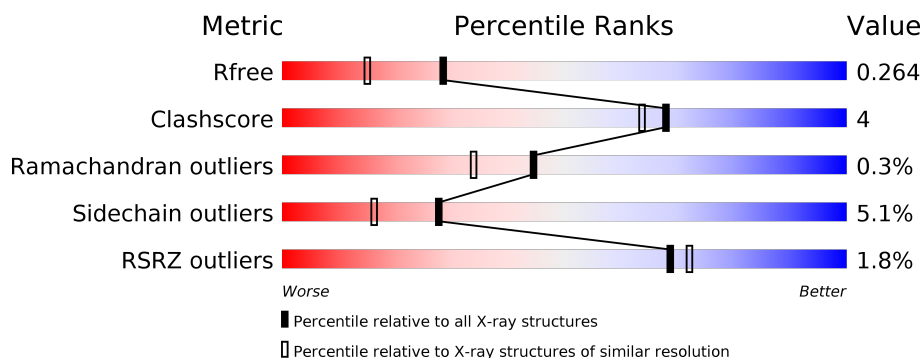
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	518	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	518	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	518	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	518	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	601	-	-	-	X
2	GOL	C	601	-	-	-	X
2	GOL	C	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17079 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3951	2493	694	731	33			
1	B	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	C	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	D	513	Total	C	N	O	S	0	0	0
			3949	2492	694	730	33			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3
A	-4	ILE	-	EXPRESSION TAG	UNP D3KVM3
A	-3	ASP	-	EXPRESSION TAG	UNP D3KVM3
A	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
A	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
A	0	THR	-	EXPRESSION TAG	UNP D3KVM3
B	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3
B	-4	ILE	-	EXPRESSION TAG	UNP D3KVM3
B	-3	ASP	-	EXPRESSION TAG	UNP D3KVM3
B	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
B	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
B	0	THR	-	EXPRESSION TAG	UNP D3KVM3
C	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3
C	-4	ILE	-	EXPRESSION TAG	UNP D3KVM3
C	-3	ASP	-	EXPRESSION TAG	UNP D3KVM3
C	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
C	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
C	0	THR	-	EXPRESSION TAG	UNP D3KVM3
D	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3
D	-4	ILE	-	EXPRESSION TAG	UNP D3KVM3
D	-3	ASP	-	EXPRESSION TAG	UNP D3KVM3

*Continued on next page...*

Continued from previous page...

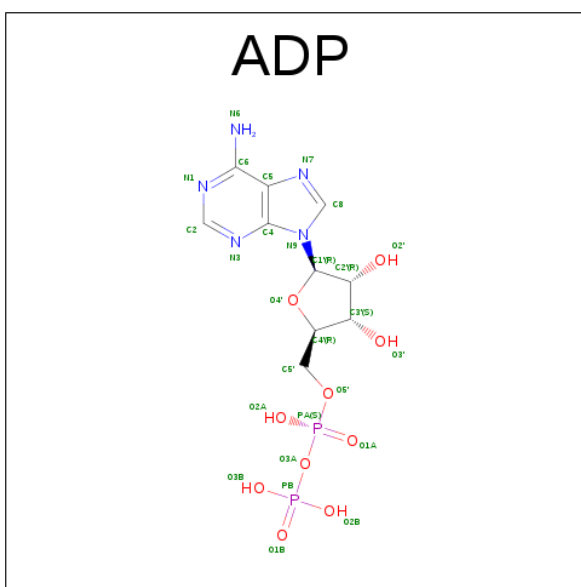
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
D	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
D	0	THR	-	EXPRESSION TAG	UNP D3KVM3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		
5	B	285	Total	O	0	0
			285	285		

*Continued on next page...*

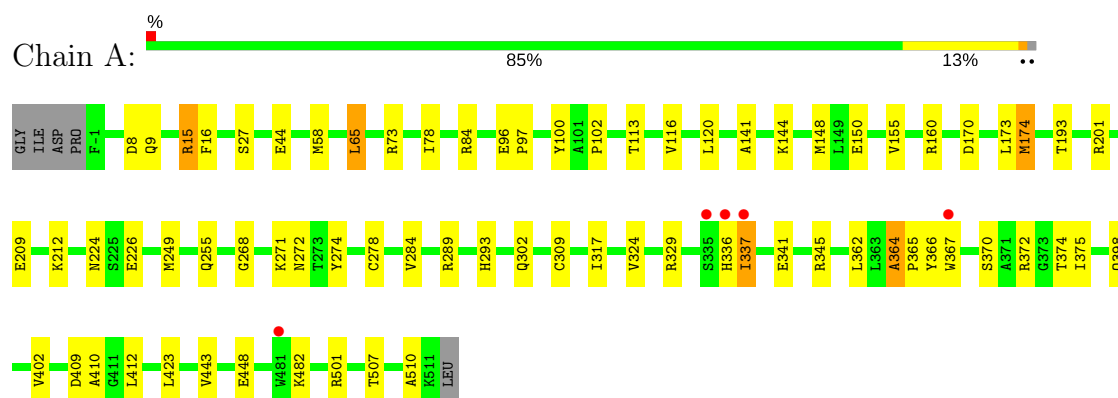
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	261	Total 261	O 261	0	0
5	D	259	Total 259	O 259	0	0

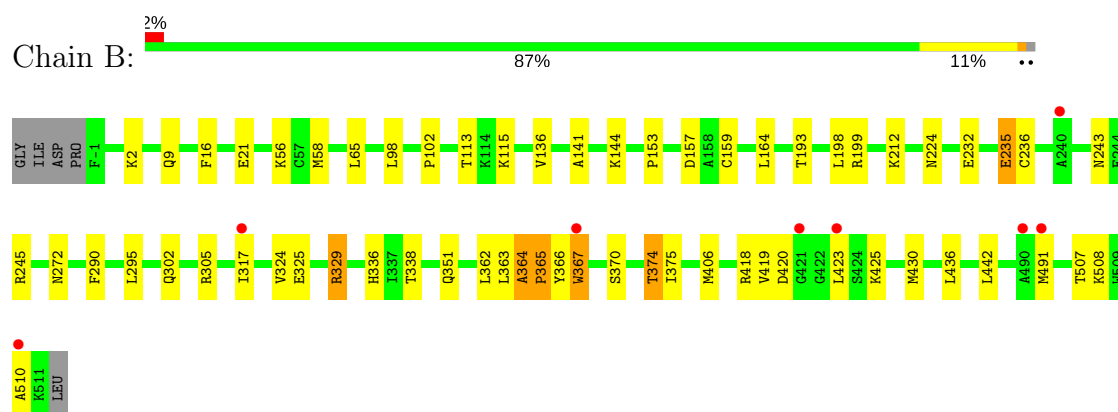
### 3 Residue-property plots [i](#)

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

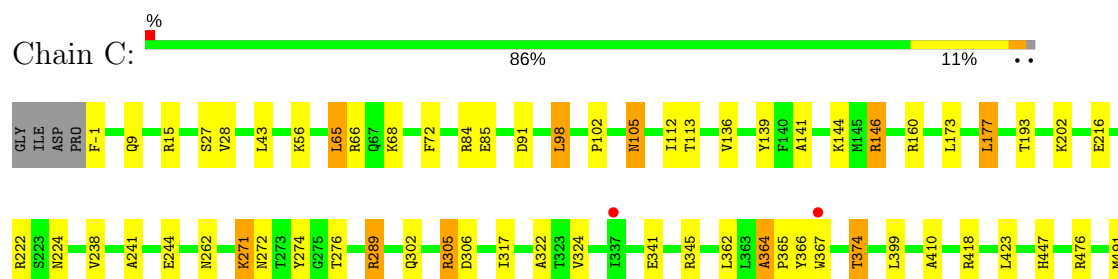
#### • Molecule 1: Glycerol kinase



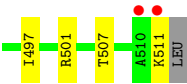
#### • Molecule 1: Glycerol kinase



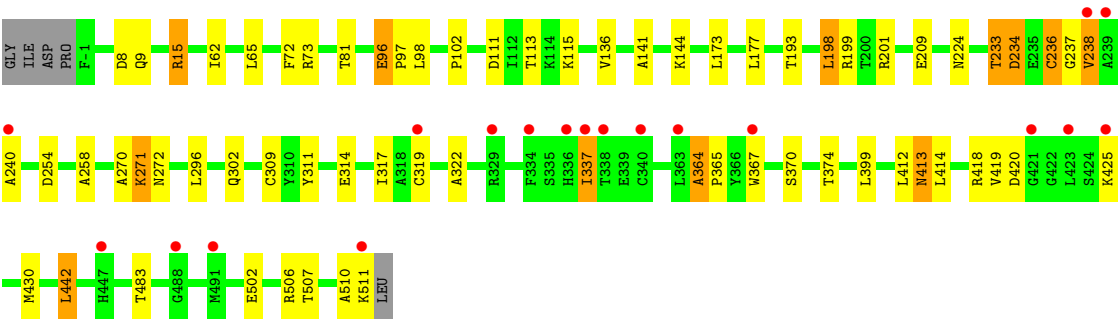
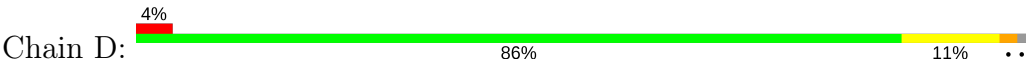
#### • Molecule 1: Glycerol kinase







● Molecule 1: Glycerol kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.12Å 153.84Å 120.10Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 31.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-1.90) 98.1 (31.56-1.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.254 0.224 , 0.264	Depositor DCC
$R_{free}$ test set	8660 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l	Xtriage
Reported twinning fraction	0.515 for H, K, L 0.485 for H, -K, -L	Depositor
Outliers	1 of 173946 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: GOL, MG, ADP

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	0.37	0/4032	0.48	0/5456
1	B	0.35	1/4039 (0.0%)	0.52	0/5465
1	C	0.44	1/4039 (0.0%)	0.51	0/5465
1	D	0.38	1/4030 (0.0%)	0.52	1/5453 (0.0%)
All	All	0.38	3/16140 (0.0%)	0.51	1/21839 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	PRO	N-CD	5.74	1.55	1.47
1	D	236	CYS	CB-SG	-5.21	1.73	1.81
1	C	238	VAL	CB-CG1	-5.21	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	GLY	N-CA-C	-5.76	98.70	113.10

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	A	3951	0	3963	42	0
1	B	3957	0	3970	30	0
1	C	3957	0	3970	37	0
1	D	3949	0	3958	36	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
2	C	18	0	24	2	0
2	D	6	0	8	0	0
3	A	27	0	12	1	0
3	B	54	0	24	0	0
3	D	54	0	24	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	287	0	0	0	0
5	B	285	0	0	2	0
5	C	261	0	0	0	0
5	D	259	0	0	1	0
All	All	17079	0	15969	142	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 4.

All (142) 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:C:364:ALA:HB1	1:C:365:PRO:HD2	1.34	1.08
1:D:364:ALA:HB1	1:D:365:PRO:HD2	1.35	1.06
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.98	0.93
1:C:364:ALA:HB1	1:C:365:PRO:CD	1.98	0.93
1:D:236:CYS:O	1:D:236:CYS:SG	2.29	0.91
1:A:364:ALA:HB1	1:A:365:PRO:HD2	1.53	0.89
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.03	0.89
1:D:317:ILE:HB	5:D:878:HOH:O	1.78	0.82
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.62	0.81
1:C:364:ALA:CB	1:C:365:PRO:HD2	2.13	0.78
1:D:224:ASN:HD22	1:D:302:GLN:H	1.28	0.78
1:B:224:ASN:HD22	1:B:302:GLN:H	1.31	0.76
1:A:364:ALA:CB	1:A:365:PRO:HD2	2.16	0.76
1:C:289:ARG:HG2	1:C:410:ALA:HA	1.66	0.75
1:A:224:ASN:HD22	1:A:302:GLN:H	1.34	0.75
1:A:364:ALA:CB	1:A:365:PRO:CD	2.66	0.72
1:C:305:ARG:HG3	1:C:305:ARG:HH11	1.56	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASN:HD22	1:C:302:GLN:H	1.37	0.70
1:B:364:ALA:CB	1:B:365:PRO:CD	2.70	0.69
1:C:113:THR:HG23	1:C:136:VAL:HG12	1.73	0.69
1:C:15:ARG:HH21	1:C:28:VAL:HG21	1.57	0.69
1:A:278:CYS:HB2	1:A:317:ILE:HG12	1.75	0.69
1:C:305:ARG:HG3	1:C:305:ARG:NH1	2.08	0.69
1:A:96:GLU:HG3	1:A:97:PRO:HD2	1.75	0.67
1:C:43:LEU:HD23	1:C:105:ASN:HD21	1.59	0.67
1:D:364:ALA:CB	1:D:365:PRO:HD2	2.19	0.66
1:A:27:SER:HB2	1:A:65:LEU:HG	1.78	0.64
1:D:113:THR:HG23	1:D:136:VAL:HG12	1.80	0.64
1:B:324:VAL:HG21	1:B:423:LEU:HD21	1.79	0.63
1:D:374:THR:HG21	1:D:507:THR:HA	1.81	0.63
1:A:374:THR:HG21	1:A:507:THR:HA	1.81	0.63
1:C:105:ASN:HD22	1:C:105:ASN:H	1.47	0.62
1:A:212:LYS:HB2	1:C:306:ASP:OD2	2.00	0.61
1:D:258:ALA:HB3	1:D:271:LYS:HD2	1.82	0.61
1:D:337:ILE:H	1:D:337:ILE:HD13	1.66	0.60
1:C:364:ALA:CB	1:C:365:PRO:CD	2.72	0.60
1:B:351:GLN:HG2	5:B:948:HOH:O	2.03	0.59
1:A:255:GLN:HE22	3:A:602:ADP:HN62	1.51	0.58
1:C:91:ASP:HB2	1:C:98:LEU:HD11	1.86	0.58
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.84	0.58
1:C:374:THR:HG21	1:C:507:THR:HG22	1.87	0.57
1:B:364:ALA:O	1:B:367:TRP:CZ3	2.58	0.56
1:D:419:VAL:HG21	1:D:430:MET:SD	2.46	0.56
1:A:102:PRO:HB2	1:A:144:LYS:HD3	1.87	0.56
1:A:84:ARG:HH21	2:A:601:GOL:H11	1.70	0.56
1:D:96:GLU:HG3	1:D:97:PRO:HD2	1.86	0.56
1:D:102:PRO:HB2	1:D:144:LYS:HD3	1.88	0.55
1:D:8:ASP:HB3	1:D:15:ARG:CG	2.37	0.54
1:A:272:ASN:HD21	1:A:278:CYS:HB3	1.73	0.54
1:C:305:ARG:CG	1:C:305:ARG:HH11	2.21	0.54
1:B:199:ARG:HD2	1:B:290:PHE:HZ	1.72	0.54
1:B:272:ASN:HB3	1:B:419:VAL:HG12	1.90	0.53
1:C:222:ARG:HA	1:C:305:ARG:HH12	1.74	0.53
1:C:271:LYS:HG2	1:C:272:ASN:N	2.19	0.52
1:A:44:GLU:OE1	1:A:100:TYR:HB2	2.09	0.52
1:A:370:SER:HA	1:A:510:ALA:HB3	1.91	0.52
1:A:289:ARG:HD3	1:A:410:ALA:HA	1.92	0.52
1:A:44:GLU:HG2	1:A:100:TYR:HB2	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:SER:HB2	1:C:65:LEU:HG	1.92	0.51
1:D:370:SER:HA	1:D:510:ALA:HB3	1.92	0.51
1:A:443:VAL:HB	1:A:482:LYS:HB3	1.93	0.51
1:D:296:LEU:HB2	1:D:314:GLU:HB3	1.93	0.51
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.29	0.51
1:C:324:VAL:HG21	1:C:423:LEU:HD21	1.93	0.50
1:D:319:CYS:HA	1:D:322:ALA:HB3	1.93	0.50
1:B:325:GLU:HG3	1:B:329:ARG:HG2	1.94	0.50
1:C:262:ASN:O	1:C:418:ARG:HD3	2.11	0.50
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.93	0.50
1:B:2:LYS:HG2	1:B:21:GLU:OE2	2.11	0.50
1:A:170:ASP:O	1:A:174:MET:HB2	2.13	0.49
1:A:341:GLU:OE2	1:A:345:ARG:NH2	2.43	0.49
1:C:374:THR:CG2	1:C:507:THR:HG22	2.42	0.49
1:A:116:VAL:HG13	1:A:120:LEU:HD12	1.94	0.49
1:B:113:THR:HG23	1:B:136:VAL:HG12	1.94	0.48
1:D:234:ASP:HA	1:D:238:VAL:HA	1.94	0.48
1:D:510:ALA:O	1:D:511:LYS:HB2	2.13	0.48
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.91	0.48
1:A:398:GLN:O	1:A:402:VAL:HG23	2.13	0.48
1:B:16:PHE:CD2	1:B:58:MET:HA	2.48	0.48
1:D:62:ILE:HG23	1:D:72:PHE:HE1	1.79	0.47
1:A:226:GLU:O	1:A:249:MET:HA	2.15	0.47
1:B:374:THR:HG21	1:B:507:THR:HG22	1.94	0.47
1:C:224:ASN:ND2	1:C:302:GLN:H	2.10	0.47
1:C:84:ARG:HH21	2:C:601:GOL:H11	1.79	0.47
1:B:418:ARG:HE	1:B:442:LEU:HD23	1.79	0.47
1:C:66:ARG:NH2	1:C:241:ALA:O	2.47	0.47
1:D:141:ALA:HB3	1:D:193:THR:HA	1.96	0.47
1:D:233:THR:O	1:D:234:ASP:HB2	2.15	0.46
1:D:8:ASP:HB3	1:D:15:ARG:HG3	1.98	0.46
1:D:272:ASN:HB3	1:D:419:VAL:HG12	1.97	0.46
1:A:148:MET:HB3	1:A:155:VAL:HG11	1.98	0.46
1:A:372:ARG:O	1:A:374:THR:HG23	2.16	0.46
1:B:159:CYS:HB2	1:B:164:LEU:HD22	1.98	0.45
1:D:8:ASP:HB3	1:D:15:ARG:HG2	1.97	0.45
1:A:364:ALA:HB1	1:A:402:VAL:HG22	1.99	0.45
1:D:198:LEU:HD22	1:D:311:TYR:HE1	1.82	0.45
1:A:8:ASP:HB3	1:A:15:ARG:HG3	1.98	0.45
1:D:442:LEU:HD12	1:D:483:THR:HG22	1.97	0.45
1:A:84:ARG:HH21	2:A:601:GOL:C1	2.30	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLU:HA	1:B:236:CYS:HA	1.77	0.45
1:A:324:VAL:HG21	1:A:423:LEU:HD21	1.98	0.45
1:D:111:ASP:O	1:D:115:LYS:HG2	2.17	0.45
1:C:102:PRO:HB2	1:C:144:LYS:HD3	1.99	0.44
1:C:497:ILE:O	1:C:501:ARG:HG2	2.16	0.44
1:A:268:GLY:HA2	1:A:412:LEU:HD13	1.99	0.44
1:A:375:ILE:HD12	1:B:375:ILE:HD12	1.98	0.44
1:C:276:THR:HG23	1:C:322:ALA:HB2	1.99	0.44
1:D:238:VAL:C	1:D:240:ALA:H	2.21	0.44
1:B:363:LEU:O	1:B:364:ALA:C	2.55	0.43
1:D:413:ASN:HD22	1:D:414:LEU:H	1.65	0.43
1:D:201:ARG:HD3	1:D:309:CYS:SG	2.58	0.43
1:A:293:HIS:HD2	1:A:409:ASP:OD2	2.00	0.43
1:B:370:SER:HB2	1:B:510:ALA:HB2	2.01	0.42
1:B:374:THR:CG2	1:B:507:THR:HG22	2.50	0.42
1:B:102:PRO:HB2	1:B:144:LYS:HD3	2.01	0.42
1:B:199:ARG:HD3	5:B:701:HOH:O	2.18	0.42
1:C:173:LEU:O	1:C:177:LEU:HB2	2.20	0.42
1:B:364:ALA:HB3	1:B:365:PRO:CD	2.48	0.42
1:A:141:ALA:HB3	1:A:193:THR:HA	2.02	0.42
1:D:198:LEU:HD22	1:D:311:TYR:CE1	2.53	0.42
1:C:85:GLU:HB3	1:C:139:TYR:O	2.19	0.42
1:A:58:MET:HE1	1:A:78:ILE:HD11	2.01	0.42
1:B:153:PRO:O	1:B:157:ASP:HB2	2.19	0.42
1:B:317:ILE:HD13	1:B:364:ALA:HB2	2.00	0.42
1:C:341:GLU:O	1:C:345:ARG:HG3	2.20	0.42
1:C:141:ALA:HB3	1:C:193:THR:HA	2.02	0.41
1:C:85:GLU:OE1	2:C:601:GOL:H12	2.21	0.41
1:B:141:ALA:HB3	1:B:193:THR:HA	2.01	0.41
1:D:234:ASP:CA	1:D:238:VAL:HA	2.50	0.41
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.55	0.41
1:D:270:ALA:HB3	1:D:414:LEU:HD11	2.02	0.41
1:A:336:HIS:ND1	1:A:337:ILE:HD13	2.36	0.41
1:B:336:HIS:HD2	1:B:338:THR:H	1.68	0.41
1:D:81:THR:OG1	1:D:254:ASP:HA	2.20	0.41
1:A:284:VAL:HB	1:A:289:ARG:HG3	2.03	0.41
1:A:16:PHE:CD2	1:A:58:MET:HA	2.56	0.41
1:B:295:LEU:HD13	1:B:406:MET:HG2	2.03	0.41
1:A:201:ARG:HD3	1:A:309:CYS:SG	2.60	0.41
1:B:419:VAL:HG21	1:B:430:MET:SD	2.61	0.41
1:D:502:GLU:HG3	1:D:506:ARG:HH12	1.84	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:HG21	1:C:146:ARG:HG2	2.02	0.40
1:A:150:GLU:O	1:C:202:LYS:HG3	2.21	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	511/518 (99%)	496 (97%)	14 (3%)	1 (0%)	51	41
1	B	511/518 (99%)	491 (96%)	19 (4%)	1 (0%)	51	41
1	C	511/518 (99%)	495 (97%)	15 (3%)	1 (0%)	51	41
1	D	511/518 (99%)	489 (96%)	19 (4%)	3 (1%)	28	16
All	All	2044/2072 (99%)	1971 (96%)	67 (3%)	6 (0%)	44	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA
1	C	364	ALA
1	D	364	ALA
1	D	367	TRP
1	D	238	VAL

### 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	420/425 (99%)	403 (96%)	17 (4%)	36	25
1	B	421/425 (99%)	399 (95%)	22 (5%)	27	16
1	C	421/425 (99%)	396 (94%)	25 (6%)	23	12
1	D	419/425 (99%)	397 (95%)	22 (5%)	26	15
All	All	1681/1700 (99%)	1595 (95%)	86 (5%)	28	16

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	ARG
1	A	65	LEU
1	A	73	ARG
1	A	113	THR
1	A	160	ARG
1	A	173	LEU
1	A	174	MET
1	A	209	GLU
1	A	271	LYS
1	A	329	ARG
1	A	337	ILE
1	A	362	LEU
1	A	366	TYR
1	A	367	TRP
1	A	448	GLU
1	A	501	ARG
1	B	9	GLN
1	B	56	LYS
1	B	65	LEU
1	B	98	LEU
1	B	115	LYS
1	B	198	LEU
1	B	212	LYS
1	B	232	GLU
1	B	235	GLU
1	B	243	ASN
1	B	245	ARG
1	B	305	ARG
1	B	329	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	362	LEU
1	B	366	TYR
1	B	367	TRP
1	B	374	THR
1	B	420	ASP
1	B	425	LYS
1	B	436	LEU
1	B	491	MET
1	B	508	LYS
1	C	-1	PHE
1	C	9	GLN
1	C	56	LYS
1	C	65	LEU
1	C	68	LYS
1	C	98	LEU
1	C	105	ASN
1	C	146	ARG
1	C	160	ARG
1	C	177	LEU
1	C	216	GLU
1	C	244	GLU
1	C	271	LYS
1	C	289	ARG
1	C	305	ARG
1	C	317	ILE
1	C	362	LEU
1	C	366	TYR
1	C	367	TRP
1	C	374	THR
1	C	399	LEU
1	C	447	HIS
1	C	476	ARG
1	C	491	MET
1	C	511	LYS
1	D	9	GLN
1	D	15	ARG
1	D	65	LEU
1	D	73	ARG
1	D	96	GLU
1	D	98	LEU
1	D	173	LEU
1	D	177	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	198	LEU
1	D	199	ARG
1	D	209	GLU
1	D	233	THR
1	D	234	ASP
1	D	271	LYS
1	D	337	ILE
1	D	399	LEU
1	D	412	LEU
1	D	413	ASN
1	D	418	ARG
1	D	420	ASP
1	D	425	LYS
1	D	442	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	30	GLN
1	A	224	ASN
1	A	272	ASN
1	A	293	HIS
1	A	302	GLN
1	B	23	GLN
1	B	224	ASN
1	B	243	ASN
1	B	302	GLN
1	B	336	HIS
1	B	447	HIS
1	C	23	GLN
1	C	36	HIS
1	C	105	ASN
1	C	224	ASN
1	C	272	ASN
1	C	302	GLN
1	C	336	HIS
1	C	447	HIS
1	D	23	GLN
1	D	29	HIS
1	D	224	ASN
1	D	302	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	351	GLN
1	D	413	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
2	GOL	A	601	-	5,5,5	0.34	0	5,5,5	0.29	0
3	ADP	A	602	-	25,29,29	1.04	1 (4%)	24,45,45	1.71	2 (8%)
2	GOL	B	601	-	5,5,5	0.31	0	5,5,5	0.31	0
3	ADP	B	602	4	25,29,29	1.05	1 (4%)	24,45,45	1.62	2 (8%)
3	ADP	B	603	4	25,29,29	1.01	1 (4%)	24,45,45	1.72	3 (12%)
2	GOL	C	601	-	5,5,5	0.36	0	5,5,5	0.15	0
2	GOL	C	602	-	5,5,5	0.34	0	5,5,5	0.27	0
2	GOL	C	603	-	5,5,5	0.35	0	5,5,5	0.27	0
2	GOL	D	601	-	5,5,5	0.36	0	5,5,5	0.22	0
3	ADP	D	602	4	25,29,29	1.01	1 (4%)	24,45,45	1.71	3 (12%)
3	ADP	D	603	4	25,29,29	1.06	1 (4%)	24,45,45	1.70	2 (8%)

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	GOL	A	601	-	-	0/4/4/4	0/0/0/0
3	ADP	A	602	-	-	0/12/32/32	0/3/3/3
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
3	ADP	B	602	4	-	0/12/32/32	0/3/3/3
3	ADP	B	603	4	-	0/12/32/32	0/3/3/3
2	GOL	C	601	-	-	0/4/4/4	0/0/0/0
2	GOL	C	602	-	-	0/4/4/4	0/0/0/0
2	GOL	C	603	-	-	0/4/4/4	0/0/0/0
2	GOL	D	601	-	-	0/4/4/4	0/0/0/0
3	ADP	D	602	4	-	0/12/32/32	0/3/3/3
3	ADP	D	603	4	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ADP	C5-C4	3.11	1.47	1.40
3	D	602	ADP	C5-C4	3.21	1.47	1.40
3	D	603	ADP	C5-C4	3.28	1.47	1.40
3	B	602	ADP	C5-C4	3.29	1.47	1.40
3	A	602	ADP	C5-C4	3.34	1.48	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ADP	N3-C2-N1	-6.67	123.05	128.86
3	D	602	ADP	N3-C2-N1	-6.54	123.16	128.86
3	D	603	ADP	N3-C2-N1	-6.41	123.28	128.86
3	A	602	ADP	N3-C2-N1	-6.24	123.42	128.86
3	B	602	ADP	N3-C2-N1	-6.22	123.44	128.86
3	D	603	ADP	C4-C5-N7	-2.84	106.67	109.41
3	D	602	ADP	C4-C5-N7	-2.83	106.67	109.41
3	A	602	ADP	C4-C5-N7	-2.79	106.72	109.41
3	B	603	ADP	C4-C5-N7	-2.64	106.86	109.41
3	B	602	ADP	C4-C5-N7	-2.63	106.87	109.41
3	D	602	ADP	C2-N1-C6	2.03	122.32	118.77
3	B	603	ADP	C2-N1-C6	2.05	122.36	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	2	0
3	A	602	ADP	1	0
2	C	601	GOL	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

### 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, 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	513/518 (99%)	0.21	5 (0%) 82 84	19, 32, 40, 44	1 (0%)
1	B	513/518 (99%)	0.20	8 (1%) 72 75	19, 31, 42, 48	1 (0%)
1	C	513/518 (99%)	0.19	4 (0%) 86 87	21, 32, 44, 51	1 (0%)
1	D	513/518 (99%)	0.29	19 (3%) 42 46	21, 33, 45, 50	1 (0%)
All	All	2052/2072 (99%)	0.22	36 (1%) 69 72	19, 32, 42, 51	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	511	LYS	4.1
1	C	367	TRP	3.9
1	C	510	ALA	3.6
1	B	423	LEU	3.6
1	D	319	CYS	3.6
1	D	421	GLY	3.4
1	B	490	ALA	3.4
1	D	240	ALA	3.2
1	D	491	MET	3.2
1	B	510	ALA	3.1
1	D	238	VAL	3.0
1	C	337	ILE	2.9
1	A	367	TRP	2.8
1	D	447	HIS	2.8
1	D	363	LEU	2.7
1	B	421	GLY	2.7
1	D	336	HIS	2.7
1	C	511	LYS	2.6
1	D	338	THR	2.6
1	D	423	LEU	2.5
1	A	336	HIS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	425	LYS	2.5
1	D	340	CYS	2.5
1	D	367	TRP	2.3
1	D	337	ILE	2.3
1	B	367	TRP	2.2
1	D	239	ALA	2.2
1	D	329	ARG	2.2
1	A	481	TRP	2.1
1	B	317	ILE	2.1
1	B	491	MET	2.1
1	A	335	SER	2.1
1	B	240	ALA	2.1
1	D	334	PHE	2.0
1	D	488	GLY	2.0
1	A	337	ILE	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. 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
2	GOL	C	601	6/6	0.75	0.24	6.12	56,57,57,57	0
2	GOL	A	601	6/6	0.74	0.21	4.74	39,40,41,41	0
2	GOL	C	603	6/6	0.80	0.28	4.43	76,76,76,76	0
3	ADP	B	602	27/27	0.93	0.14	0.90	41,44,45,45	0
3	ADP	A	602	27/27	0.84	0.13	0.68	60,60,61,61	0
2	GOL	C	602	6/6	0.90	0.13	0.66	49,49,49,49	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	D	603	27/27	0.94	0.11	0.57	34,35,36,37	0
2	GOL	D	601	6/6	0.96	0.10	-0.38	25,26,26,26	0
3	ADP	D	602	27/27	0.95	0.10	-0.50	33,33,39,40	0
2	GOL	B	601	6/6	0.95	0.10	-0.51	26,26,26,27	0
3	ADP	B	603	27/27	0.96	0.10	-0.67	29,29,30,30	0
4	MG	B	604	1/1	0.94	0.07	-	32,32,32,32	0
4	MG	D	604	1/1	0.91	0.06	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.