



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:41 AM GMT

PDB ID : 1EYZ  
Title : STRUCTURE OF ESCHERICHIA COLI PURT-ENCODED GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE COMPLEXED WITH MG AND AMPPNP  
Authors : Thoden, J.B.; Firestone, S.; Nixon, A.; Benkovic, S.J.; Holden, H.M.  
Deposited on : 2000-05-09  
Resolution : 1.75 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

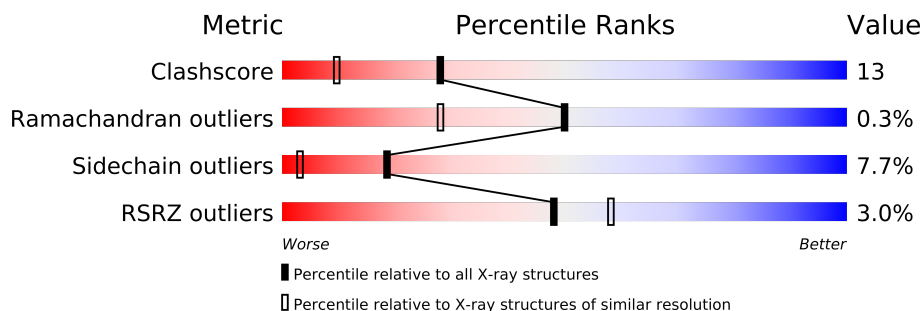
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.75 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))
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NA	A	961	-	X
3	NA	B	960	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6878 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHORIBOSYLGLYCINAMIDEFORMYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2970	1870	529	558	13			
1	B	389	Total	C	N	O	S	0	2	0
			2979	1875	534	557	13			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	3	Total	Mg	0	0
			3	3		

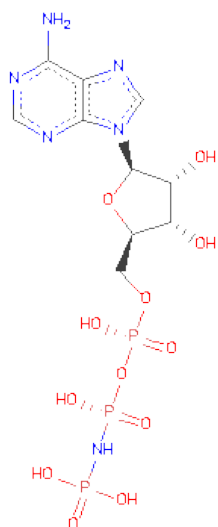
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

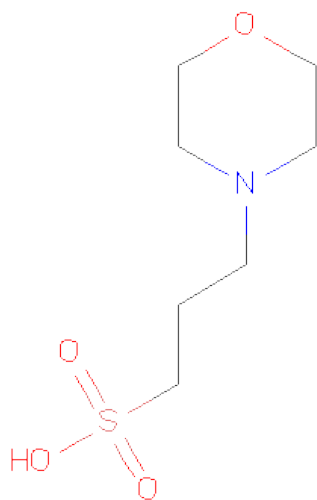
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is 3[N-MORPHOLINO]PROPANESULFONIC ACID (three-letter code: MPO) (formula:  $C_7H_{15}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is water.

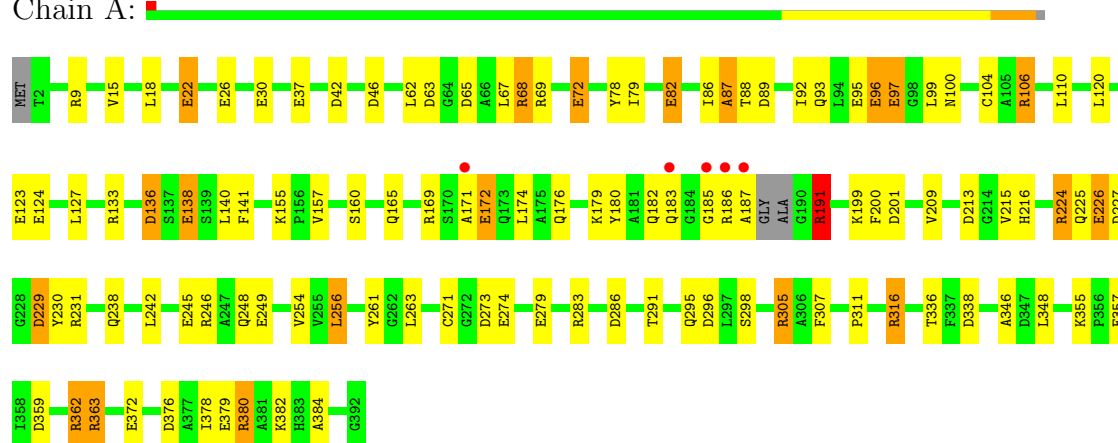
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	488	Total 488	O 488	0	0
7	B	358	Total 358	O 358	0	0

### 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.

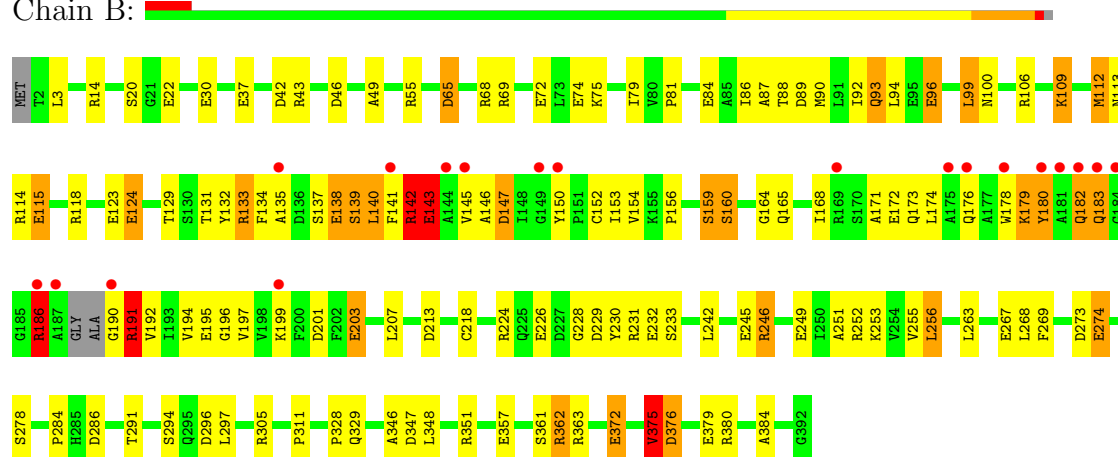
#### • Molecule 1: PHOSPHORIBOSYLGLYCINAMIDEFORMYLTRANSFERASE 2

Chain A:



#### • Molecule 1: PHOSPHORIBOSYLGLYCINAMIDEFORMYLTRANSFERASE 2

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.30Å 179.50Å 75.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 31.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-1.75) 93.7 (31.11-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.89 (at 1.70Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.185 , 0.228 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 92.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 88307 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, MPO, ANP, 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	0.95	21/3023 (0.7%)	1.33	45/4095 (1.1%)
1	B	0.99	26/3036 (0.9%)	1.29	35/4111 (0.9%)
All	All	0.97	47/6059 (0.8%)	1.31	80/8206 (1.0%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	GLU	CD-OE2	9.36	1.35	1.25
1	B	138	GLU	CD-OE2	8.67	1.35	1.25
1	B	138	GLU	CD-OE1	-8.02	1.16	1.25
1	B	84	GLU	CD-OE2	7.75	1.34	1.25
1	B	379	GLU	CD-OE2	7.56	1.33	1.25
1	B	124	GLU	CD-OE2	7.00	1.33	1.25
1	B	249	GLU	CD-OE2	6.88	1.33	1.25
1	A	30	GLU	CD-OE2	6.66	1.32	1.25
1	A	379	GLU	CD-OE2	6.62	1.32	1.25
1	A	249	GLU	CD-OE2	6.60	1.32	1.25
1	B	245	GLU	CD-OE2	6.57	1.32	1.25
1	B	123	GLU	CD-OE1	-6.54	1.18	1.25
1	A	274	GLU	CD-OE2	6.48	1.32	1.25
1	B	226	GLU	CD-OE2	6.28	1.32	1.25
1	A	97	GLU	CD-OE2	6.11	1.32	1.25
1	A	279	GLU	CD-OE2	6.08	1.32	1.25
1	A	124	GLU	CD-OE2	5.97	1.32	1.25
1	B	172	GLU	CD-OE2	5.85	1.32	1.25
1	B	22	GLU	CD-OE2	5.81	1.32	1.25
1	A	138	GLU	CD-OE2	5.79	1.32	1.25
1	B	143	GLU	CD-OE2	5.75	1.31	1.25
1	A	123	GLU	CD-OE2	5.75	1.31	1.25
1	A	22	GLU	CD-OE2	5.69	1.31	1.25
1	A	72	GLU	CD-OE2	5.68	1.31	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLU	CD-OE2	5.68	1.31	1.25
1	A	26	GLU	CD-OE2	5.63	1.31	1.25
1	B	372	GLU	CD-OE2	5.58	1.31	1.25
1	B	203	GLU	CD-OE2	5.57	1.31	1.25
1	A	82	GLU	CD-OE2	5.50	1.31	1.25
1	A	37	GLU	CD-OE2	5.49	1.31	1.25
1	B	284	PRO	N-CD	5.47	1.55	1.47
1	B	274	GLU	CD-OE2	5.47	1.31	1.25
1	B	267	GLU	CD-OE2	5.45	1.31	1.25
1	A	172	GLU	CD-OE2	5.45	1.31	1.25
1	B	357	GLU	CD-OE2	5.44	1.31	1.25
1	B	72	GLU	CD-OE2	5.44	1.31	1.25
1	A	96	GLU	CD-OE2	5.40	1.31	1.25
1	A	245	GLU	CD-OE2	5.31	1.31	1.25
1	B	195	GLU	CD-OE2	5.30	1.31	1.25
1	B	30	GLU	CD-OE2	5.29	1.31	1.25
1	A	357	GLU	CD-OE2	5.29	1.31	1.25
1	A	226	GLU	CD-OE2	5.20	1.31	1.25
1	B	115	GLU	CD-OE2	5.13	1.31	1.25
1	A	95	GLU	CD-OE2	5.07	1.31	1.25
1	B	96	GLU	CD-OE2	5.07	1.31	1.25
1	B	232	GLU	CD-OE1	-5.06	1.20	1.25
1	B	84	GLU	CD-OE1	-5.03	1.20	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	286	ASP	CB-CG-OD2	-8.93	110.27	118.30
1	A	380	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	191	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	286	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	376	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	147	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	213	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	363	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	316	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	338	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	42	ASP	CB-CG-OD1	7.18	124.76	118.30
1	B	347	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	B	42	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	201	ASP	CB-CG-OD2	-7.03	111.97	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	296	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	296	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	286	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	238	GLN	N-CA-CB	-6.75	98.46	110.60
1	A	227	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	213	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	89	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	180	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	A	338	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	136	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	227	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	68	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	147	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	376	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	201	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	305	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	65	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	201	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	89	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	359	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	286	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	201	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	133	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	191	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	351	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	233	SER	N-CA-CB	5.79	119.19	110.50
1	B	273	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	63	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	273	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	261	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	B	191	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	65	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	89	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	69	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	46	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	359	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	65	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	89	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	42	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	186	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	229	ASP	CB-CG-OD2	-5.41	113.43	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	296	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	224	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	273	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	375	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	A	46	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	42	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	380	ARG	CD-NE-CZ	5.27	130.97	123.60
1	B	246	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	65	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	283	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	213	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	104	CYS	N-CA-CB	5.24	120.03	110.60
1	B	351	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	305	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	9	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	363	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	133	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	118	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	142	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	136	ASP	N-CA-CB	5.02	119.64	110.60
1	A	172	GLU	CB-CG-CD	-5.02	100.64	114.20
1	B	213	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2992	55	0
1	B	2979	0	3006	96	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	31	0	13	1	0
5	B	31	0	13	3	0
6	A	13	0	15	1	0
7	A	488	0	0	18	0
7	B	358	0	0	9	1
All	All	6878	0	6039	153	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:79:ILE:HD11	1:B:99:LEU:HD22	1.31	1.08
1:B:115:GLU:HG3	1:B:134:PHE:CE1	2.01	0.95
1:B:191:ARG:HG3	1:B:192:VAL:N	1.82	0.94
1:B:173:GLN:HA	1:B:176:GLN:NE2	1.85	0.91
1:B:380[B]:ARG:HH11	1:B:380[B]:ARG:HG2	1.36	0.90
1:B:153:ILE:HD12	1:B:197:VAL:HG22	1.51	0.89
1:B:68:ARG:HE	1:B:90:MET:HE1	1.41	0.83
1:B:156:PRO:HG2	1:B:159:SER:HB2	1.61	0.81
1:A:291:THR:HB	7:A:2002:HOH:O	1.80	0.81
1:B:145:VAL:HG13	1:B:152:CYS:SG	2.22	0.79
1:B:141:PHE:O	1:B:145:VAL:HG23	1.83	0.78
1:B:68:ARG:HB2	1:B:90:MET:HE3	1.67	0.77
1:B:79:ILE:HD11	1:B:99:LEU:CD2	2.12	0.76
1:A:295:GLN:HB2	7:A:2002:HOH:O	1.86	0.76
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.49	0.76
1:B:153:ILE:CD1	1:B:197:VAL:HG22	2.15	0.76
1:B:132:TYR:O	1:B:133:ARG:HD2	1.89	0.73
1:B:143:GLU:O	1:B:146:ALA:HB3	1.89	0.72
1:B:65:ASP:O	1:B:69:ARG:HG3	1.91	0.71
1:A:298:SER:HA	7:A:2002:HOH:O	1.91	0.71
1:A:79:ILE:HD11	1:A:99:LEU:HD23	1.73	0.69
1:A:362:ARG:NH1	7:A:1375:HOH:O	2.26	0.69
1:B:178:TRP:O	1:B:182:GLN:NE2	2.26	0.68
1:B:68:ARG:HB2	1:B:90:MET:CE	2.24	0.68
1:B:68:ARG:NE	1:B:90:MET:HE1	2.09	0.67
1:B:156:PRO:HG2	1:B:159:SER:CB	2.24	0.67
1:A:68:ARG:O	1:A:72:GLU:HG3	1.95	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:ARG:NH2	7:A:1297:HOH:O	2.28	0.66
1:B:153:ILE:HD12	1:B:197:VAL:CG2	2.24	0.65
1:A:180:TYR:O	1:A:183:GLN:HB2	1.96	0.65
1:A:199:LYS:NZ	7:A:1804:HOH:O	2.30	0.65
1:A:92:ILE:O	1:A:96:GLU:HG3	1.98	0.64
1:B:348:LEU:HB2	1:B:380[A]:ARG:NH2	2.13	0.63
1:B:228:GLY:HA2	7:B:1596:HOH:O	1.98	0.63
1:A:18:LEU:HD11	1:A:67:LEU:HD11	1.82	0.62
1:A:378:ILE:O	1:A:382:LYS:HG3	2.00	0.62
1:A:68:ARG:NH2	1:A:97:GLU:OE1	2.34	0.61
1:A:295:GLN:NE2	7:A:2002:HOH:O	2.28	0.61
1:B:93:GLN:O	1:B:96:GLU:HB3	2.01	0.60
1:A:169:ARG:NH1	7:A:1984:HOH:O	2.31	0.60
1:B:346:ALA:O	1:B:380[A]:ARG:NH2	2.34	0.60
1:B:362:ARG:NH2	7:B:1642:HOH:O	2.35	0.59
1:B:173:GLN:O	1:B:176:GLN:HB2	2.01	0.59
1:B:174:LEU:N	1:B:174:LEU:HD23	2.16	0.59
1:B:274:GLU:HB3	7:B:2046:HOH:O	2.01	0.59
1:A:79:ILE:HD11	1:A:99:LEU:CD2	2.32	0.59
1:B:138:GLU:OE1	1:B:142:ARG:NH1	2.36	0.59
1:B:380[B]:ARG:HG2	1:B:380[B]:ARG:NH1	2.11	0.58
1:B:94:LEU:HB3	1:B:99:LEU:HD13	1.87	0.56
1:A:136:ASP:HB3	1:A:191:ARG:HD3	1.88	0.56
1:A:216:HIS:HD2	7:A:1811:HOH:O	1.89	0.56
1:B:68:ARG:CB	1:B:90:MET:HE3	2.34	0.56
1:A:183:GLN:HB3	7:A:1803:HOH:O	2.06	0.55
1:B:81:PRO:HB3	1:B:86:ILE:CD1	2.36	0.55
1:A:86:ILE:O	1:A:88:THR:HG23	2.07	0.55
1:B:88:THR:O	1:B:92:ILE:HD12	2.06	0.54
1:A:68:ARG:HD2	7:A:1316:HOH:O	2.07	0.54
1:B:180:TYR:C	1:B:182:GLN:H	2.10	0.53
1:B:115:GLU:HG3	1:B:134:PHE:CZ	2.43	0.53
1:A:171:ALA:HA	1:A:174:LEU:HG	1.91	0.53
1:A:229:ASP:HA	7:A:1394:HOH:O	2.09	0.53
1:B:380[A]:ARG:NH1	7:B:1479:HOH:O	2.21	0.53
1:B:79:ILE:CD1	1:B:99:LEU:HD22	2.23	0.52
5:B:961:ANP:O5'	5:B:961:ANP:H8	2.10	0.51
1:B:291:THR:HA	1:B:294:SER:OG	2.10	0.51
1:B:135:ALA:CB	1:B:141:PHE:HA	2.41	0.51
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.41	0.51
1:A:209:VAL:HG22	1:A:263:LEU:HD12	1.92	0.51
1:B:156:PRO:HD3	1:B:164:GLY:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:SER:HB3	1:B:49:ALA:HB3	1.92	0.50
1:B:179:LYS:O	1:B:182:GLN:HB2	2.10	0.50
1:A:86:ILE:HG22	1:A:87:ALA:N	2.26	0.50
1:B:231:ARG:NH2	7:B:1674:HOH:O	2.44	0.50
1:A:185:GLY:C	1:A:187:ALA:H	2.15	0.49
1:B:14:ARG:HG2	1:B:37:GLU:HB3	1.94	0.49
1:A:336:THR:HB	1:B:3:LEU:HD11	1.93	0.49
1:B:253:LYS:NZ	7:B:2103:HOH:O	2.46	0.49
1:B:171:ALA:O	1:B:174:LEU:HG	2.11	0.49
1:A:224:ARG:HG3	7:A:1717:HOH:O	2.12	0.49
1:B:138:GLU:O	1:B:142:ARG:HB2	2.13	0.48
1:A:15:VAL:HG22	1:A:78:TYR:HB2	1.95	0.48
1:A:127:LEU:CD1	1:A:254:VAL:HG23	2.43	0.48
5:A:400:ANP:O5'	5:A:400:ANP:H8	2.14	0.48
1:B:93:GLN:OE1	1:B:93:GLN:HA	2.11	0.48
1:B:132:TYR:HA	1:B:194:VAL:O	2.14	0.48
1:B:141:PHE:CE1	1:B:145:VAL:CG2	2.96	0.48
1:B:131:THR:OG1	1:B:196:GLY:HA3	2.13	0.48
1:B:160:SER:HA	5:B:961:ANP:O1B	2.14	0.47
1:A:172:GLU:HG3	7:A:2092:HOH:O	2.13	0.47
1:A:127:LEU:HD11	1:A:254:VAL:HG23	1.95	0.47
1:B:109:LYS:O	1:B:112:MET:HG3	2.15	0.47
1:B:203:GLU:HG3	1:B:269:PHE:CD1	2.49	0.47
1:B:114:ARG:HH22	5:B:961:ANP:PB	2.37	0.47
1:A:110:LEU:HD13	1:A:120:LEU:HD22	1.96	0.47
1:A:348:LEU:HD11	1:A:384:ALA:HB2	1.96	0.47
1:A:22:GLU:OE1	1:A:355:LYS:NZ	2.44	0.47
1:B:252:ARG:O	1:B:256:LEU:HB2	2.15	0.46
1:A:231:ARG:HD3	1:A:231:ARG:HA	1.70	0.46
1:B:154:VAL:O	1:B:165:GLN:HA	2.15	0.46
1:B:328:PRO:HD2	1:B:362:ARG:O	2.16	0.46
1:B:251:ALA:O	1:B:255:VAL:HG13	2.15	0.46
1:B:269:PHE:CE2	1:B:278:SER:HB2	2.51	0.46
1:B:88:THR:HG21	1:B:112:MET:HG2	1.98	0.45
1:B:173:GLN:HA	1:B:176:GLN:HE22	1.72	0.45
1:B:180:TYR:CD2	1:B:183:GLN:HB2	2.51	0.45
1:B:139:SER:HB3	7:B:2060:HOH:O	2.16	0.45
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.82	0.45
1:B:156:PRO:CG	1:B:159:SER:CB	2.95	0.45
1:B:380[B]:ARG:CG	1:B:380[B]:ARG:NH1	2.79	0.45
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.83	0.45
1:A:155:LYS:HG2	1:A:165:GLN:HG3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:GLU:HB2	7:A:1103:HOH:O	2.17	0.45
1:A:180:TYR:CD2	1:A:183:GLN:NE2	2.86	0.44
1:A:138:GLU:O	1:A:141:PHE:HB3	2.16	0.44
1:B:203:GLU:HG3	1:B:269:PHE:HD1	1.82	0.44
1:A:200:PHE:HA	1:A:271:CYS:SG	2.57	0.44
1:B:135:ALA:HB1	1:B:141:PHE:N	2.33	0.44
1:A:185:GLY:O	1:A:187:ALA:N	2.50	0.44
1:B:348:LEU:HD11	1:B:384:ALA:CB	2.48	0.44
1:B:252:ARG:HG3	1:B:256:LEU:HD22	2.00	0.44
1:A:256:LEU:HA	1:A:256:LEU:HD12	1.87	0.44
1:A:225:GLN:NE2	7:A:1815:HOH:O	2.51	0.44
1:B:297:LEU:HA	7:B:1554:HOH:O	2.18	0.44
1:A:22:GLU:OE2	1:A:363:ARG:NH1	2.48	0.43
1:B:329:GLN:HG2	7:B:1565:HOH:O	2.19	0.43
1:B:115:GLU:HG3	1:B:134:PHE:CD1	2.52	0.43
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.53	0.43
1:B:305:ARG:HD2	1:B:311:PRO:O	2.19	0.43
1:A:157:VAL:HG22	1:A:191:ARG:O	2.19	0.43
1:A:209:VAL:O	1:A:215:VAL:HA	2.19	0.43
1:A:242:LEU:O	1:A:246:ARG:HG3	2.19	0.43
1:B:55:ARG:HE	1:B:74:GLU:CD	2.21	0.42
1:B:348:LEU:HD11	1:B:384:ALA:HB2	2.01	0.42
1:B:150:TYR:HE2	1:B:168:ILE:HG22	1.84	0.42
1:B:137:SER:O	1:B:140:LEU:N	2.51	0.42
1:B:242:LEU:O	1:B:246:ARG:HG3	2.19	0.42
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.54	0.42
1:A:305:ARG:HD3	1:A:311:PRO:O	2.19	0.42
1:B:375:VAL:HG12	1:B:376:ASP:N	2.35	0.42
1:B:207:LEU:HB2	1:B:218:CYS:HB2	2.02	0.42
1:A:226:GLU:HB3	1:A:231:ARG:HG2	2.02	0.41
1:B:113:ASN:OD1	1:B:115:GLU:HB2	2.20	0.41
1:B:20:SER:CB	1:B:49:ALA:HB3	2.50	0.41
1:B:186:ARG:NH1	1:B:190:GLY:N	2.69	0.41
1:B:180:TYR:C	1:B:182:GLN:N	2.73	0.41
1:B:86:ILE:HG22	1:B:87:ALA:N	2.35	0.41
1:B:182:GLN:NE2	1:B:182:GLN:N	2.69	0.41
1:A:346:ALA:O	1:A:380:ARG:NH1	2.54	0.41
6:A:950:MPO:H72	7:A:1204:HOH:O	2.21	0.41
1:B:180:TYR:HD2	1:B:183:GLN:HB2	1.86	0.40
1:B:156:PRO:HB2	1:B:159:SER:HB3	2.03	0.40
1:B:154:VAL:O	1:B:165:GLN:HG3	2.22	0.40
1:A:248:GLN:NE2	7:A:2091:HOH:O	2.48	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	Distance(Å)	Clash(Å)
7:B:1663:HOH:O	7:B:1663:HOH:O[2.655]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	386/392 (98%)	371 (96%)	13 (3%)	2 (0%)	38	15
1	B	387/392 (99%)	371 (96%)	16 (4%)	0	100	100
All	All	773/784 (99%)	742 (96%)	29 (4%)	2 (0%)	50	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	A	87	ALA

### 5.3.2 Protein sidechains ⓘ

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	312/312 (100%)	296 (95%)	16 (5%)	33	9
1	B	313/312 (100%)	279 (89%)	34 (11%)	9	1
All	All	625/624 (100%)	575 (92%)	50 (8%)	18	2

All (50) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	93[A]	GLN
1	A	93[B]	GLN
1	A	100	ASN
1	A	106	ARG
1	A	140	LEU
1	A	160	SER
1	A	176	GLN
1	A	179	LYS
1	A	182	GLN
1	A	191	ARG
1	A	224	ARG
1	A	230	TYR
1	A	256	LEU
1	A	307	PHE
1	A	316	ARG
1	A	362	ARG
1	B	43[A]	ARG
1	B	43[B]	ARG
1	B	75	LYS
1	B	93	GLN
1	B	99	LEU
1	B	100	ASN
1	B	106	ARG
1	B	109	LYS
1	B	112	MET
1	B	124	GLU
1	B	129	THR
1	B	133	ARG
1	B	139	SER
1	B	140	LEU
1	B	142	ARG
1	B	143	GLU
1	B	147	ASP
1	B	159	SER
1	B	160	SER
1	B	179	LYS
1	B	182	GLN
1	B	183	GLN
1	B	186	ARG
1	B	191	ARG
1	B	199	LYS
1	B	229	ASP
1	B	230	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	256	LEU
1	B	263	LEU
1	B	268	LEU
1	B	361	SER
1	B	362	ARG
1	B	372	GLU
1	B	375	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	182	GLN
1	A	183	GLN
1	A	216	HIS
1	A	225	GLN
1	A	248	GLN
1	A	329	GLN
1	B	100	ASN
1	B	176	GLN
1	B	182	GLN
1	B	225	GLN
1	B	248	GLN
1	B	329	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ANP	A	400	2	33,33,33	1.44	6 (18%)	51,52,52	1.55	6 (11%)
6	MPO	A	950	-	13,13,13	1.86	2 (15%)	17,17,17	2.63	5 (29%)
5	ANP	B	961	2	33,33,33	1.82	6 (18%)	51,52,52	1.44	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	A	400	2	-	0/18/38/38	0/1/3/3
6	MPO	A	950	-	-	0/7/15/15	0/1/1/1
5	ANP	B	961	2	-	0/18/38/38	0/1/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	961	ANP	PG-N3B	-5.65	1.59	1.64
5	B	961	ANP	PB-N3B	-5.37	1.59	1.64
6	A	950	MPO	C3-N1	4.27	1.57	1.47
6	A	950	MPO	C1-S1	4.09	1.83	1.77
5	A	400	ANP	PG-O1G	3.75	1.50	1.46
5	B	961	ANP	PB-O1B	3.33	1.50	1.46
5	A	400	ANP	PB-O1B	3.11	1.50	1.46
5	B	961	ANP	PG-O1G	2.89	1.49	1.46
5	B	961	ANP	C6-N6	-2.81	1.26	1.35
5	A	400	ANP	C6-N6	-2.61	1.26	1.35
5	A	400	ANP	PG-N3B	-2.60	1.62	1.64
5	B	961	ANP	C2-N1	2.51	1.38	1.33
5	A	400	ANP	PG-O3G	2.31	1.62	1.55
5	A	400	ANP	PB-N3B	-2.08	1.62	1.64

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	950	MPO	O1-S1-C1	7.44	113.18	106.81
5	A	400	ANP	N3-C2-N1	-5.95	123.73	128.71
6	A	950	MPO	O3-S1-O1	-5.08	100.81	111.78
5	B	961	ANP	N3-C2-N1	-4.79	124.71	128.71
5	A	400	ANP	O1G-PG-N3B	-4.66	104.79	111.83
5	A	400	ANP	C2-N1-C6	4.05	126.09	118.77
5	B	961	ANP	O4'-C1'-N9	-3.91	104.80	108.44
6	A	950	MPO	O3-S1-C1	3.82	110.76	105.93
5	A	400	ANP	C5-C6-N6	3.69	129.06	120.72
5	B	961	ANP	C5-C6-N6	3.65	128.97	120.72
5	B	961	ANP	C2-N1-C6	3.47	125.04	118.77
6	A	950	MPO	O2-S1-C1	2.83	109.24	106.81
5	B	961	ANP	O2B-PB-N3B	2.64	113.77	106.61
5	A	400	ANP	C5-C6-N1	-2.41	111.19	119.27
5	B	961	ANP	C5-C6-N1	-2.32	111.49	119.27
5	A	400	ANP	O3'-C3'-C2'	2.29	119.29	111.83
6	A	950	MPO	C2-C1-S1	-2.18	110.43	113.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	389/392 (99%)	-0.52	5 (1%) 74 84	10, 17, 49, 97	0
1	B	389/392 (99%)	-0.20	19 (4%) 28 36	11, 22, 81, 100	0
All	All	778/784 (99%)	-0.36	24 (3%) 48 56	10, 19, 70, 100	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	6.3
1	B	176	GLN	6.1
1	B	135	ALA	4.6
1	B	187	ALA	4.4
1	B	190	GLY	3.3
1	B	141	PHE	3.2
1	B	183	GLN	3.2
1	B	186	ARG	3.1
1	B	150	TYR	3.1
1	A	187	ALA	2.8
1	B	180	TYR	2.8
1	B	145	VAL	2.7
1	B	149	GLY	2.7
1	A	186	ARG	2.6
1	A	185	GLY	2.5
1	B	169	ARG	2.4
1	B	199	LYS	2.3
1	B	184	GLY	2.2
1	A	171	ALA	2.2
1	B	178	TRP	2.1
1	B	181	ALA	2.1
1	A	183	GLN	2.0
1	B	144	ALA	2.0
1	B	182	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	961	1/1	0.30	14.06	21,21,21,21	0
3	NA	B	960	1/1	0.27	10.78	37,37,37,37	0
6	MPO	A	950	13/13	0.06	-0.89	15,23,31,40	0
5	ANP	B	961	31/31	0.06	-1.07	18,28,37,62	0
5	ANP	A	400	31/31	0.04	-1.09	12,15,22,25	0
2	MG	B	401	1/1	0.02	-1.96	25,25,25,25	0
2	MG	A	403	1/1	0.04	-2.14	29,29,29,29	0
2	MG	A	401	1/1	0.05	-2.15	18,18,18,18	0
4	CL	A	970	1/1	0.04	-3.50	26,26,26,26	0
2	MG	B	402	1/1	0.03	-4.84	23,23,23,23	0
2	MG	A	402	1/1	0.02	-96.87	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.