



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2017 – 09:38 PM EDT

PDB ID : 1Q99  
Title : Crystal structure of the *Saccharomyces cerevisiae* SR protein kinsae, Sky1p, complexed with the non-hydrolyzable ATP analogue, AMP-PNP  
Authors : Nolen, B.; Ngo, J.; Chakrabarti, S.; Vu, D.; Adams, J.A.; Ghosh, G.  
Deposited on : unknown  
Resolution : 2.11 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
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) : rb-20029824

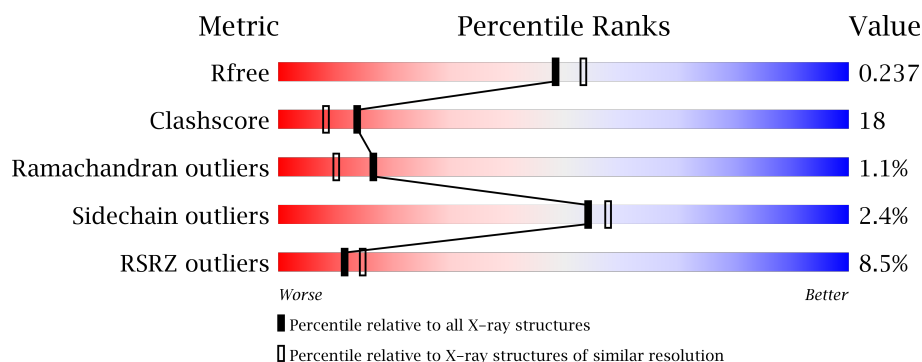
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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	373	<div> <div>8%</div> <div>62%</div> <div>31%</div> <div>• 5%</div> </div>
1	B	373	<div> <div>9%</div> <div>66%</div> <div>29%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	1439	-	-	-	X
6	MOH	B	2000	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6112 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 SR protein kinsae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2848	1829	486	521	12			
1	B	364	Total	C	N	O	S	0	0	0
			2940	1886	500	542	12			

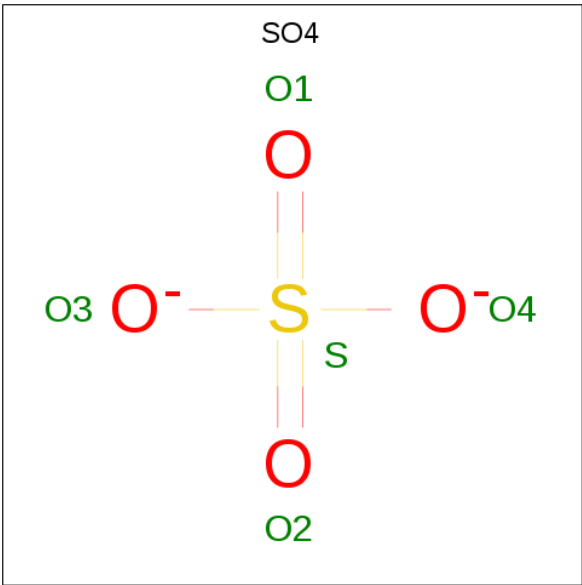
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	VAL	-	SEE REMARK 999	UNP Q03656
A	306	ASP	-	SEE REMARK 999	UNP Q03656
B	305	VAL	-	SEE REMARK 999	UNP Q03656
B	306	ASP	-	SEE REMARK 999	UNP Q03656

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

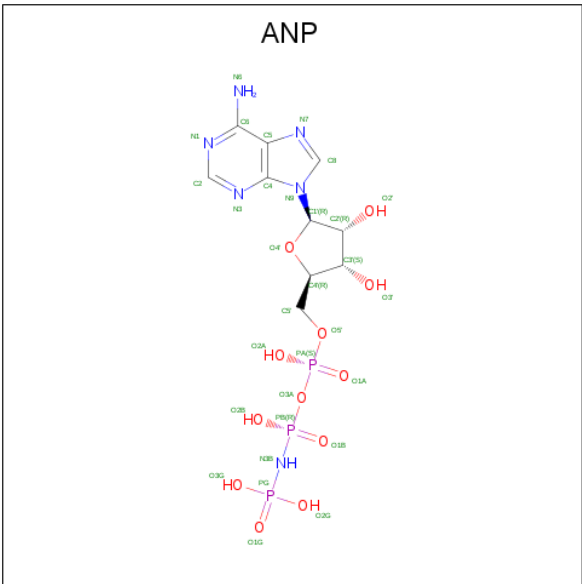
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

- 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		
3	B	1	Total	O	S	0	0
			5	4	1		

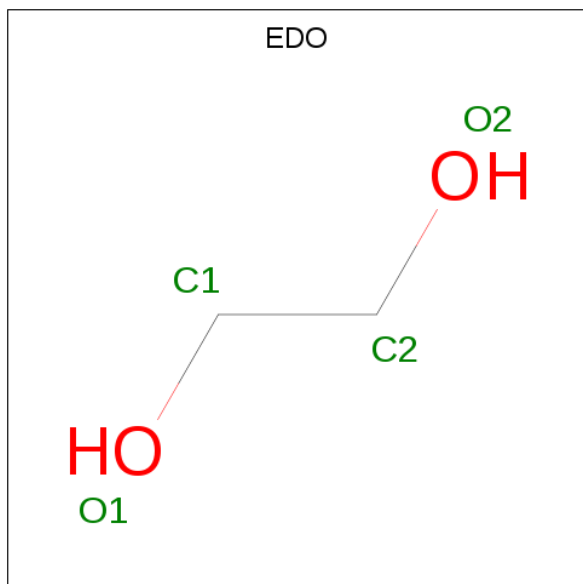
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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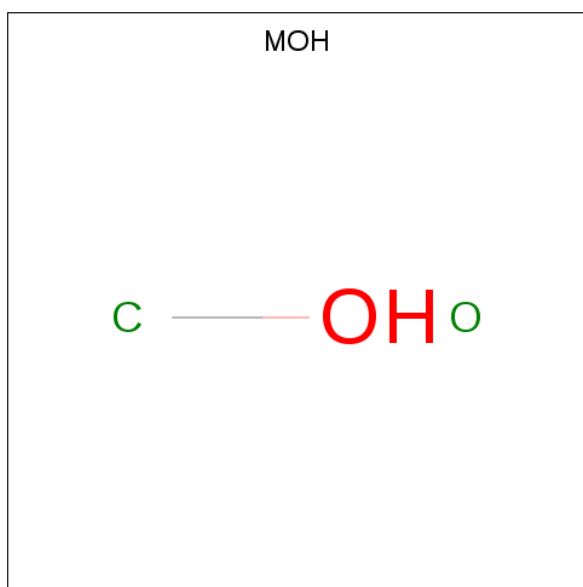
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is METHANOL (three-letter code: MOH) (formula:  $CH_4O$ ).



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

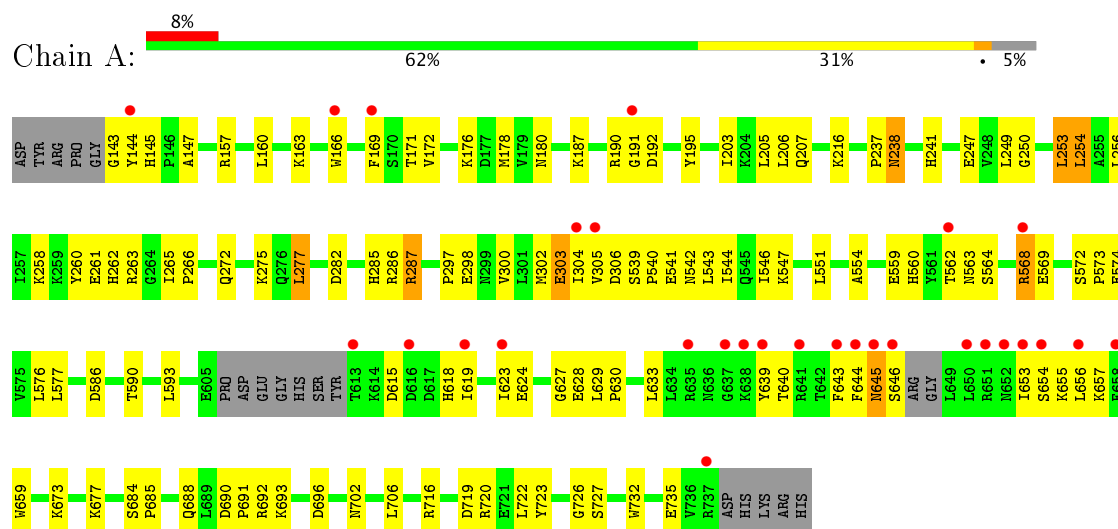
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	128	Total	O	0	0
			128	128		
7	B	110	Total	O	0	0
			110	110		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: SR protein kinsae



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.41Å 88.95Å 134.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.11 40.11 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.95-2.11) 91.9 (40.11-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, $R_{free}$	0.220 , 0.260 0.239 , 0.237	Depositor DCC
$R_{free}$ test set	2336 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.16 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.9878e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MOH, ANP, EDO, SO4

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	0.34	0/2915	0.56	0/3944
1	B	0.34	0/3013	0.57	0/4079
All	All	0.34	0/5928	0.56	0/8023

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	2848	0	2811	110	0
1	B	2940	0	2902	101	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	2	0
5	A	4	0	6	0	0
5	B	4	0	6	1	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	A	128	0	0	5	0
7	B	110	0	0	8	0
All	All	6112	0	5751	206	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 18.

All (206) 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:562:THR:HG22	1:A:564:SER:H	1.11	1.12
1:A:655:LYS:HD3	1:A:657:LYS:HE3	1.47	0.97
1:A:623:ILE:HD11	1:A:629:LEU:HD13	1.50	0.91
1:A:249:LEU:HD21	1:A:547:LYS:HD2	1.52	0.88
1:A:172:VAL:HG22	1:A:187:LYS:HG2	1.58	0.85
1:B:568:ARG:HH21	1:B:618:HIS:HD2	1.23	0.84
1:B:673:LYS:HE2	1:B:677:LYS:HE2	1.61	0.82
1:A:143:GLY:HA3	1:A:171:THR:HG23	1.62	0.81
1:B:238:ASN:H	1:B:238:ASN:ND2	1.80	0.80
1:B:282:ASP:OD1	1:B:286:ARG:HD3	1.81	0.80
1:B:650:LEU:HD23	1:B:653:ILE:HB	1.63	0.78
1:A:282:ASP:OD1	1:A:286:ARG:HD3	1.84	0.78
1:B:604:PHE:O	1:B:606:PRO:HD3	1.86	0.75
1:A:562:THR:HG22	1:A:564:SER:N	1.96	0.74
1:B:253:LEU:HD22	1:B:300:VAL:HB	1.69	0.73
1:A:624:GLU:HG3	1:A:657:LYS:O	1.89	0.72
1:B:203:ILE:O	1:B:207:GLN:HG3	1.89	0.72
1:A:623:ILE:CD1	1:A:629:LEU:HD13	2.20	0.71
1:B:238:ASN:H	1:B:238:ASN:HD22	1.37	0.71
1:B:568:ARG:HH21	1:B:618:HIS:CD2	2.05	0.70
1:B:305:VAL:HG21	1:B:545:GLN:HB2	1.73	0.69
1:A:659:TRP:HB2	1:B:657:LYS:HG2	1.75	0.69
1:B:641:ARG:HE	1:B:641:ARG:HA	1.58	0.69
1:B:238:ASN:N	1:B:238:ASN:HD22	1.89	0.68
1:A:655:LYS:HE2	1:B:659:TRP:CH2	2.30	0.67
1:B:615:ASP:HB3	1:B:643:PHE:HE2	1.59	0.66
1:B:306:ASP:OD2	1:B:540:PRO:HD2	1.95	0.65
1:B:305:VAL:CG2	1:B:545:GLN:HB2	2.26	0.65
1:A:145:HIS:HB2	1:A:241:HIS:CE1	2.31	0.65
1:A:238:ASN:ND2	1:A:238:ASN:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HD3	1:A:593:LEU:HD13	1.79	0.64
1:B:172:VAL:HG22	1:B:187:LYS:HG2	1.81	0.63
1:B:659:TRP:HB3	7:B:2033:HOH:O	1.98	0.63
1:B:615:ASP:HB3	1:B:643:PHE:CE2	2.33	0.62
1:A:304:ILE:N	1:A:304:ILE:HD12	2.14	0.62
1:A:673:LYS:HG2	1:A:677:LYS:HE2	1.81	0.62
1:A:272:GLN:HE22	1:A:543:LEU:HA	1.65	0.62
1:A:673:LYS:HE2	1:A:677:LYS:HE2	1.82	0.60
1:B:272:GLN:HE22	1:B:543:LEU:HA	1.65	0.60
1:B:272:GLN:HE22	1:B:544:ILE:H	1.49	0.60
1:A:673:LYS:HE2	1:A:677:LYS:CE	2.33	0.59
1:B:163:LYS:HE3	1:B:166:TRP:HE1	1.67	0.59
1:A:144:TYR:CB	1:A:190:ARG:HG3	2.33	0.59
1:A:702:ASN:OD1	1:A:716:ARG:HB2	2.01	0.59
1:B:247:GLU:HB3	7:B:2030:HOH:O	2.02	0.59
1:B:157:ARG:HG3	1:B:179:VAL:HG23	1.84	0.58
1:B:722:LEU:O	1:B:723:TYR:HB2	2.03	0.58
1:A:655:LYS:HA	1:B:667:GLU:OE1	2.02	0.58
1:A:272:GLN:HE22	1:A:544:ILE:H	1.53	0.57
1:B:539:SER:HB3	1:B:540:PRO:HD3	1.86	0.57
1:B:148:PHE:CZ	1:B:151:GLU:HG3	2.40	0.57
1:A:577:LEU:HD21	1:A:629:LEU:HD23	1.86	0.56
1:A:619:ILE:HD12	1:A:643:PHE:CD2	2.40	0.56
1:A:653:ILE:HD12	1:A:653:ILE:N	2.19	0.56
1:B:203:ILE:HD13	1:B:231:HIS:CD2	2.40	0.56
1:A:690:ASP:HB3	1:A:693:LYS:NZ	2.20	0.56
1:B:256:LEU:HD22	1:B:265:ILE:HD13	1.87	0.56
1:A:147:ALA:HB1	1:A:160:LEU:CD1	2.36	0.56
1:B:673:LYS:HE2	1:B:677:LYS:CE	2.35	0.55
1:A:673:LYS:O	1:A:677:LYS:HG3	2.06	0.55
1:A:145:HIS:HE1	1:A:237:PRO:HD2	1.72	0.55
1:B:187:LYS:HD3	1:B:246:PHE:CE1	2.42	0.55
4:B:902:ANP:H2'	7:B:2109:HOH:O	2.06	0.55
1:A:203:ILE:O	1:A:207:GLN:HG3	2.07	0.54
1:A:306:ASP:OD2	1:A:540:PRO:HD2	2.07	0.54
1:B:272:GLN:NE2	1:B:544:ILE:H	2.04	0.54
1:A:657:LYS:HD2	1:B:657:LYS:NZ	2.22	0.54
1:B:226:LEU:HD13	1:B:249:LEU:HD11	1.89	0.54
1:B:702:ASN:OD1	1:B:716:ARG:HB2	2.08	0.54
1:A:169:PHE:HB3	1:A:195:TYR:HE1	1.72	0.54
1:A:247:GLU:HG3	1:A:249:LEU:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD22	1:A:300:VAL:HB	1.89	0.53
1:A:574:GLU:HG2	1:A:691:PRO:HG3	1.90	0.53
1:A:576:LEU:HD11	1:A:618:HIS:CD2	2.42	0.53
1:B:226:LEU:HD13	1:B:249:LEU:CD1	2.38	0.53
1:B:645:ASN:CB	1:B:651:ARG:HH21	2.21	0.53
1:B:645:ASN:HA	1:B:651:ARG:NH2	2.23	0.53
1:B:145:HIS:HB2	1:B:241:HIS:CE1	2.43	0.53
1:B:249:LEU:HD12	1:B:301:LEU:HD12	1.91	0.53
1:A:572:SER:HB2	1:A:573:PRO:HD2	1.91	0.53
1:A:254:LEU:HG	1:A:298:GLU:OE2	2.09	0.52
1:A:304:ILE:HD12	1:A:304:ILE:H	1.72	0.52
1:B:696:ASP:CG	1:B:720:ARG:HH21	2.12	0.52
1:B:147:ALA:HB1	1:B:160:LEU:CD1	2.40	0.52
1:B:645:ASN:HB3	1:B:651:ARG:HH21	1.74	0.52
1:A:629:LEU:HG	1:A:633:LEU:HD12	1.92	0.52
1:B:546:ILE:C	1:B:546:ILE:HD12	2.29	0.52
1:B:584:GLY:HA3	7:B:2027:HOH:O	2.09	0.52
1:A:247:GLU:HG3	1:A:249:LEU:HD13	1.91	0.52
1:A:629:LEU:HG	1:A:633:LEU:CD1	2.40	0.52
1:B:256:LEU:HD22	1:B:265:ILE:CD1	2.40	0.52
1:B:666:THR:HG22	1:B:667:GLU:N	2.25	0.52
1:B:572:SER:HB2	1:B:574:GLU:OE2	2.10	0.52
1:A:205:LEU:HD13	1:A:554:ALA:HB3	1.92	0.52
1:A:176:LYS:HD3	1:A:178:MET:HE1	1.93	0.51
1:A:560:HIS:HE1	7:A:2095:HOH:O	1.93	0.51
1:A:539:SER:HB3	1:A:540:PRO:HD3	1.92	0.51
1:A:238:ASN:N	1:A:238:ASN:HD22	2.07	0.51
1:A:238:ASN:N	1:A:238:ASN:ND2	2.57	0.51
1:A:654:SER:HB2	7:A:2061:HOH:O	2.10	0.51
1:B:249:LEU:HD11	1:B:547:LYS:HD2	1.93	0.51
1:B:277:LEU:CD1	1:B:590:THR:HG23	2.40	0.50
1:A:163:LYS:HE2	1:A:166:TRP:NE1	2.26	0.50
1:A:272:GLN:NE2	1:A:544:ILE:H	2.08	0.50
1:A:655:LYS:HD3	1:A:657:LYS:CE	2.29	0.50
1:A:645:ASN:HD22	1:A:645:ASN:C	2.15	0.50
1:B:630:PRO:HD2	1:B:633:LEU:HD12	1.93	0.50
1:A:256:LEU:HB2	1:A:302:MET:CE	2.42	0.50
1:A:287:ARG:HD2	7:A:2081:HOH:O	2.11	0.50
1:B:657:LYS:HB2	1:B:657:LYS:NZ	2.26	0.50
1:A:261:GLU:O	1:A:263:ARG:HG3	2.11	0.50
1:A:256:LEU:HB2	1:A:302:MET:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:HD22	1:B:300:VAL:CB	2.40	0.49
1:A:238:ASN:H	1:A:238:ASN:HD22	1.61	0.49
1:A:690:ASP:HB3	1:A:693:LYS:HZ3	1.77	0.49
1:A:298:GLU:H	1:A:298:GLU:CD	2.15	0.49
1:B:643:PHE:O	1:B:651:ARG:HG2	2.13	0.49
1:A:157:ARG:HH21	1:A:180:ASN:ND2	2.11	0.48
1:A:655:LYS:HG3	1:B:659:TRP:CZ2	2.47	0.48
1:A:277:LEU:HD13	1:A:590:THR:HG23	1.96	0.48
1:B:252:ASN:OD1	1:B:254:LEU:HB2	2.13	0.48
1:A:688:GLN:NE2	1:A:693:LYS:NZ	2.60	0.48
1:A:722:LEU:O	1:A:723:TYR:HB2	2.14	0.48
1:B:604:PHE:C	1:B:606:PRO:HD3	2.34	0.48
1:A:696:ASP:HA	1:A:732:TRP:CH2	2.49	0.48
1:A:645:ASN:ND2	1:A:646:SER:N	2.62	0.47
1:A:562:THR:HG22	1:A:563:ASN:N	2.28	0.47
1:A:275:LYS:HD2	1:A:706:LEU:HB3	1.95	0.47
1:A:169:PHE:HB2	1:A:195:TYR:CD1	2.49	0.47
1:B:688:GLN:HE21	1:B:690:ASP:H	1.62	0.47
1:B:297:PRO:HD3	1:B:593:LEU:HD13	1.97	0.47
1:A:639:TYR:N	1:A:639:TYR:CD1	2.83	0.47
1:B:143:GLY:HA2	1:B:190:ARG:HE	1.79	0.46
1:A:216:LYS:HG3	7:A:2118:HOH:O	2.14	0.46
1:A:254:LEU:HD12	1:A:298:GLU:HG3	1.96	0.46
1:B:645:ASN:HA	1:B:651:ARG:HH21	1.80	0.46
1:A:656:LEU:N	1:B:667:GLU:OE1	2.49	0.46
5:B:1439:EDO:H11	7:B:2008:HOH:O	2.16	0.46
1:A:192:ASP:HB3	1:A:195:TYR:HB2	1.97	0.46
1:A:630:PRO:HB3	7:A:2057:HOH:O	2.15	0.45
1:A:684:SER:HB2	1:A:685:PRO:HD3	1.98	0.45
1:B:297:PRO:HG2	1:B:298:GLU:OE1	2.17	0.45
1:A:657:LYS:HD2	1:B:657:LYS:HZ3	1.81	0.45
1:B:690:ASP:CB	1:B:693:LYS:HE3	2.48	0.44
1:A:305:VAL:HG13	1:A:306:ASP:N	2.33	0.44
1:A:640:THR:O	1:A:644:PHE:HD1	1.99	0.44
1:A:191:GLY:HA3	1:A:241:HIS:CE1	2.53	0.44
1:A:615:ASP:HB3	1:A:643:PHE:CE2	2.53	0.44
1:B:170:SER:HB2	1:B:188:ILE:O	2.18	0.44
1:B:226:LEU:HD21	4:B:902:ANP:HN61	1.83	0.44
1:B:254:LEU:HD12	1:B:298:GLU:HG3	1.99	0.44
1:A:302:MET:C	1:A:303:GLU:OE2	2.56	0.44
1:B:254:LEU:O	1:B:258:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ILE:C	1:A:546:ILE:HD12	2.39	0.43
1:B:163:LYS:CE	1:B:166:TRP:HE1	2.31	0.43
1:B:285:HIS:HE1	1:B:586:ASP:OD2	2.01	0.43
1:A:302:MET:HG3	1:A:303:GLU:N	2.32	0.43
1:B:147:ALA:HB1	1:B:160:LEU:HD11	2.00	0.43
1:B:576:LEU:HD21	1:B:618:HIS:CG	2.53	0.43
1:B:641:ARG:NE	1:B:641:ARG:HA	2.32	0.43
1:B:251:GLU:HG3	7:B:2059:HOH:O	2.17	0.43
1:A:256:LEU:HG	1:A:265:ILE:HD13	2.00	0.43
1:B:298:GLU:N	1:B:298:GLU:OE1	2.51	0.43
1:A:254:LEU:O	1:A:258:LYS:HG3	2.18	0.43
1:A:304:ILE:H	1:A:304:ILE:CD1	2.32	0.43
1:B:202:GLU:HA	1:B:205:LEU:HD12	2.01	0.43
1:B:180:ASN:O	1:B:182:THR:HG23	2.19	0.43
1:B:302:MET:O	1:B:303:GLU:HB3	2.18	0.43
1:A:623:ILE:HD12	1:A:628:GLU:HA	2.00	0.43
1:B:595:PHE:CD1	1:B:603:LEU:HD13	2.53	0.43
1:B:578:GLY:HA2	7:B:2103:HOH:O	2.18	0.42
1:B:302:MET:C	1:B:303:GLU:OE1	2.57	0.42
1:A:306:ASP:HB3	1:A:543:LEU:HB2	2.00	0.42
1:A:577:LEU:HD21	1:A:629:LEU:CD2	2.48	0.42
1:B:206:LEU:HD23	1:B:551:LEU:HD12	2.00	0.42
1:A:692:ARG:O	1:A:727:SER:HB3	2.20	0.42
1:A:568:ARG:HB3	1:A:569:GLU:OE1	2.20	0.42
1:B:171:THR:HG22	7:B:2047:HOH:O	2.18	0.42
1:B:596:GLU:HA	1:B:601:ASP:O	2.20	0.42
1:B:576:LEU:HD21	1:B:618:HIS:CD2	2.55	0.42
1:B:593:LEU:O	1:B:593:LEU:HD12	2.20	0.42
1:A:285:HIS:HE1	1:A:586:ASP:OD2	2.02	0.42
1:A:623:ILE:HD13	1:A:627:GLY:O	2.19	0.42
1:A:726:GLY:HA3	1:A:732:TRP:CE2	2.55	0.42
1:A:304:ILE:N	1:A:304:ILE:CD1	2.81	0.42
1:A:559:GLU:HA	1:A:735:GLU:OE2	2.20	0.42
1:B:591:ALA:HB2	1:B:686:MET:HB3	2.02	0.42
1:A:260:TYR:CE2	1:A:266:PRO:HD3	2.55	0.41
1:B:192:ASP:HB3	1:B:195:TYR:HB2	2.03	0.41
1:B:574:GLU:HG2	1:B:691:PRO:HG3	2.02	0.41
1:B:626:LEU:HD12	1:B:689:LEU:HD21	2.02	0.41
1:B:571:ARG:HD3	1:B:575:VAL:HG12	2.02	0.41
1:B:292:HIS:C	1:B:293:THR:HG23	2.41	0.41
1:B:645:ASN:CA	1:B:651:ARG:HH21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:O	1:A:303:GLU:HB3	2.20	0.41
1:A:690:ASP:HA	1:A:691:PRO:HD2	1.84	0.41
1:A:541:GLU:O	1:A:542:ASN:HB2	2.21	0.41
1:A:615:ASP:HB3	1:A:643:PHE:HE2	1.86	0.41
1:B:163:LYS:HZ2	1:B:166:TRP:HZ2	1.68	0.41
1:A:298:GLU:CD	1:A:298:GLU:N	2.75	0.40
1:B:218:ASP:OD1	1:B:287:ARG:HG2	2.21	0.40
1:B:642:THR:O	1:B:651:ARG:HD2	2.21	0.40
1:A:206:LEU:HD23	1:A:551:LEU:HD12	2.02	0.40
1:A:722:LEU:HG	1:A:723:TYR:CD1	2.57	0.40
1:A:719:ASP:O	1:A:720:ARG:HD2	2.22	0.40
1:B:663:ASP:HB3	1:B:667:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

## 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	348/373 (93%)	324 (93%)	20 (6%)	4 (1%)	17	10
1	B	362/373 (97%)	339 (94%)	19 (5%)	4 (1%)	17	10
All	All	710/746 (95%)	663 (93%)	39 (6%)	8 (1%)	17	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	568	ARG
1	A	262	HIS
1	A	568	ARG
1	B	250	GLY
1	B	303	GLU
1	B	654	SER

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Mol	Chain	Res	Type
1	A	303	GLU
1	A	250	GLY

### 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	305/327 (93%)	299 (98%)	6 (2%)	60	65
1	B	317/327 (97%)	308 (97%)	9 (3%)	49	51
All	All	622/654 (95%)	607 (98%)	15 (2%)	54	58

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

Mol	Chain	Res	Type
1	A	238	ASN
1	A	253	LEU
1	A	254	LEU
1	A	277	LEU
1	A	287	ARG
1	A	645	ASN
1	B	238	ASN
1	B	253	LEU
1	B	277	LEU
1	B	287	ARG
1	B	576	LEU
1	B	641	ARG
1	B	666	THR
1	B	714	GLU
1	B	737	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN

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Mol	Chain	Res	Type
1	A	238	ASN
1	A	272	GLN
1	A	285	HIS
1	A	560	HIS
1	A	618	HIS
1	A	645	ASN
1	A	688	GLN
1	B	145	HIS
1	B	224	HIS
1	B	231	HIS
1	B	238	ASN
1	B	272	GLN
1	B	285	HIS
1	B	618	HIS
1	B	621	GLN
1	B	636	ASN
1	B	688	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	EDO	A	1440	-	3,3,3	0.62	0	2,2,2	0.40	0
6	MOH	A	2001	6	1,1,1	0.45	0	0,0,0	0.00	-
3	SO4	A	801	-	4,4,4	0.38	0	6,6,6	0.10	0
4	ANP	A	901	-	29,33,33	1.58	5 (17%)	28,52,52	2.29	5 (17%)
5	EDO	B	1439	-	3,3,3	0.60	0	2,2,2	0.43	0
6	MOH	B	2000	6	1,1,1	0.44	0	0,0,0	0.00	-
3	SO4	B	802	-	4,4,4	0.37	0	6,6,6	0.09	0
4	ANP	B	902	-	29,33,33	1.59	5 (17%)	28,52,52	2.31	5 (17%)

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	EDO	A	1440	-	-	0/1/1/1	0/0/0/0
6	MOH	A	2001	6	-	0/0/0/0	0/0/0/0
3	SO4	A	801	-	-	0/0/0/0	0/0/0/0
4	ANP	A	901	-	-	0/13/38/38	0/3/3/3
5	EDO	B	1439	-	-	0/1/1/1	0/0/0/0
6	MOH	B	2000	6	-	0/0/0/0	0/0/0/0
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0
4	ANP	B	902	-	-	0/13/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ANP	PG-O2G	-2.98	1.48	1.56
4	B	902	ANP	PG-O2G	-2.98	1.48	1.56
4	B	902	ANP	PB-O2B	-2.70	1.49	1.56
4	A	901	ANP	PB-O2B	-2.70	1.49	1.56
4	A	901	ANP	PG-O1G	2.02	1.48	1.46
4	A	901	ANP	PB-O1B	2.13	1.48	1.46
4	B	902	ANP	PB-O1B	2.16	1.48	1.46
4	B	902	ANP	PG-O1G	2.20	1.48	1.46
4	A	901	ANP	O4'-C1'	5.47	1.48	1.41
4	B	902	ANP	O4'-C1'	5.48	1.48	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	ANP	N3-C2-N1	-9.55	120.54	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ANP	N3-C2-N1	-9.41	120.66	128.86
4	A	901	ANP	PA-O3A-PB	-3.17	121.19	132.38
4	B	902	ANP	PA-O3A-PB	-3.01	121.75	132.38
4	B	902	ANP	O1B-PB-N3B	-2.59	107.92	111.79
4	A	901	ANP	O1B-PB-N3B	-2.50	108.05	111.79
4	A	901	ANP	O3G-PG-O1G	-2.23	107.74	113.41
4	B	902	ANP	O3G-PG-O1G	-2.22	107.77	113.41
4	A	901	ANP	O2B-PB-O1B	4.07	118.33	109.87
4	B	902	ANP	O2B-PB-O1B	4.15	118.50	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1439	EDO	1	0
4	B	902	ANP	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	354/373 (94%)	0.43	29 (8%) 12 16	13, 30, 59, 73	0
1	B	364/373 (97%)	0.47	32 (8%) 11 14	12, 29, 58, 71	0
All	All	718/746 (96%)	0.45	61 (8%) 11 15	12, 29, 59, 73	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	641	ARG	8.5
1	B	648	GLY	8.1
1	A	613	THR	6.7
1	A	305	VAL	6.6
1	B	646	SER	6.0
1	A	169	PHE	5.2
1	A	304	ILE	4.9
1	A	166	TRP	4.8
1	B	649	LEU	4.8
1	B	611	SER	4.6
1	B	647	ARG	4.5
1	A	654	SER	4.4
1	B	143	GLY	4.4
1	B	304	ILE	4.3
1	B	142	GLY	4.3
1	B	612	TYR	4.3
1	A	616	ASP	4.2
1	B	305	VAL	4.2
1	B	654	SER	4.1
1	A	658	PHE	4.1
1	B	653	ILE	4.1
1	A	644	PHE	3.9
1	B	166	TRP	3.9
1	B	613	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	609	GLY	3.8
1	A	653	ILE	3.7
1	B	655	LYS	3.5
1	A	637	GLY	3.5
1	A	651	ARG	3.5
1	B	634	LEU	3.5
1	B	610	HIS	3.4
1	B	737	ARG	3.4
1	B	650	LEU	3.4
1	A	646	SER	3.3
1	B	641	ARG	3.2
1	B	607	ASP	3.2
1	A	656	LEU	3.2
1	A	639	TYR	3.1
1	B	608	GLU	3.0
1	A	623	ILE	2.9
1	A	635	ARG	2.9
1	A	650	LEU	2.9
1	A	737	ARG	2.8
1	B	645	ASN	2.8
1	A	638	LYS	2.8
1	A	619	ILE	2.7
1	B	614	LYS	2.7
1	B	169	PHE	2.7
1	A	562	THR	2.5
1	A	645	ASN	2.5
1	A	144	TYR	2.5
1	A	652	ASN	2.5
1	B	644	PHE	2.4
1	B	639	TYR	2.4
1	A	643	PHE	2.4
1	B	658	PHE	2.3
1	B	576	LEU	2.2
1	A	568	ARG	2.2
1	B	539	SER	2.2
1	B	657	LYS	2.2
1	A	191	GLY	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 [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( $\text{\AA}^2$ )	Q<0.9
6	MOH	B	2000	2/2	0.75	0.21	4.64	40,40,40,42	0
5	EDO	B	1439	4/4	0.88	0.24	2.21	41,43,43,43	0
3	SO4	B	802	5/5	0.71	0.19	1.55	71,73,73,74	0
6	MOH	A	2001	2/2	0.78	0.14	1.46	42,42,42,44	0
5	EDO	A	1440	4/4	0.79	0.23	1.03	41,41,43,44	0
3	SO4	A	801	5/5	0.84	0.16	0.77	54,55,58,59	0
4	ANP	B	902	31/31	0.90	0.12	-0.47	32,41,44,45	0
4	ANP	A	901	31/31	0.93	0.11	-0.58	29,37,39,41	0
2	NI	B	363	1/1	0.99	0.05	-1.81	30,30,30,30	0
2	NI	A	362	1/1	0.98	0.04	-2.41	39,39,39,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.