



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:53 AM UTC

PDB ID : 4NSN / pdb_00004nsn
Title : Crystal structure of purine nucleoside phosphorylase from *Porphyromonas gingivalis* ATCC 33277, NYSGRC Target 030972, orthorhombic symmetry
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2013-11-28
Resolution : 1.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

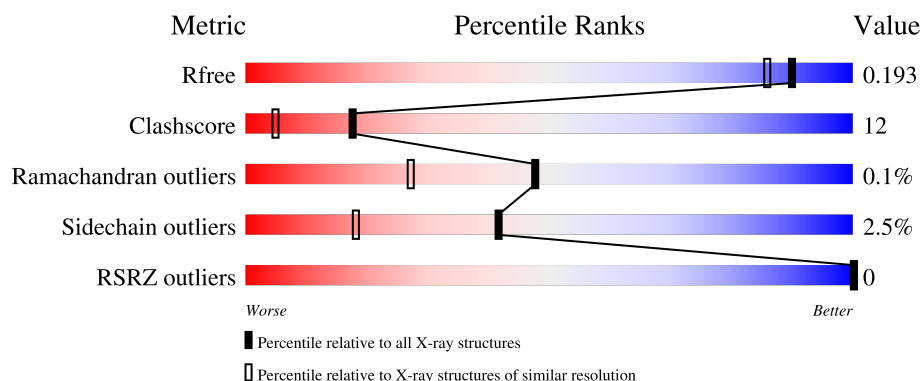
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	
1	B	295	
1	C	295	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADE	A	301	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6724 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	Se	0	9	0
			2131	1365	359	394	1	12			
1	B	273	Total	C	N	O	S	Se	0	9	0
			2131	1365	359	394	1	12			
1	C	273	Total	C	N	O	S	Se	0	8	0
			2127	1360	359	396	1	11			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MSE	-	expression tag	UNP B2RKN6
A	-5	HIS	-	expression tag	UNP B2RKN6
A	-4	HIS	-	expression tag	UNP B2RKN6
A	-3	HIS	-	expression tag	UNP B2RKN6
A	-2	HIS	-	expression tag	UNP B2RKN6
A	-1	HIS	-	expression tag	UNP B2RKN6
A	0	HIS	-	expression tag	UNP B2RKN6
A	1	SER	-	expression tag	UNP B2RKN6
A	2	SER	-	expression tag	UNP B2RKN6
A	3	GLY	-	expression tag	UNP B2RKN6
A	4	VAL	-	expression tag	UNP B2RKN6
A	5	ASP	-	expression tag	UNP B2RKN6
A	6	LEU	-	expression tag	UNP B2RKN6
A	7	GLY	-	expression tag	UNP B2RKN6
A	8	THR	-	expression tag	UNP B2RKN6
A	9	GLU	-	expression tag	UNP B2RKN6
A	10	ASN	-	expression tag	UNP B2RKN6
A	11	LEU	-	expression tag	UNP B2RKN6
A	12	TYR	-	expression tag	UNP B2RKN6
A	13	PHE	-	expression tag	UNP B2RKN6
A	14	GLN	-	expression tag	UNP B2RKN6
A	15	SER	-	expression tag	UNP B2RKN6
B	-6	MSE	-	expression tag	UNP B2RKN6

Continued on next page...

Continued from previous page...

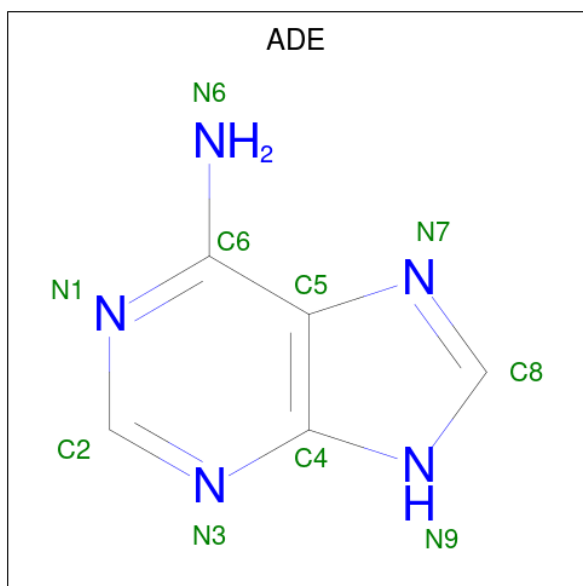
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP B2RKN6
B	-4	HIS	-	expression tag	UNP B2RKN6
B	-3	HIS	-	expression tag	UNP B2RKN6
B	-2	HIS	-	expression tag	UNP B2RKN6
B	-1	HIS	-	expression tag	UNP B2RKN6
B	0	HIS	-	expression tag	UNP B2RKN6
B	1	SER	-	expression tag	UNP B2RKN6
B	2	SER	-	expression tag	UNP B2RKN6
B	3	GLY	-	expression tag	UNP B2RKN6
B	4	VAL	-	expression tag	UNP B2RKN6
B	5	ASP	-	expression tag	UNP B2RKN6
B	6	LEU	-	expression tag	UNP B2RKN6
B	7	GLY	-	expression tag	UNP B2RKN6
B	8	THR	-	expression tag	UNP B2RKN6
B	9	GLU	-	expression tag	UNP B2RKN6
B	10	ASN	-	expression tag	UNP B2RKN6
B	11	LEU	-	expression tag	UNP B2RKN6
B	12	TYR	-	expression tag	UNP B2RKN6
B	13	PHE	-	expression tag	UNP B2RKN6
B	14	GLN	-	expression tag	UNP B2RKN6
B	15	SER	-	expression tag	UNP B2RKN6
C	-6	MSE	-	expression tag	UNP B2RKN6
C	-5	HIS	-	expression tag	UNP B2RKN6
C	-4	HIS	-	expression tag	UNP B2RKN6
C	-3	HIS	-	expression tag	UNP B2RKN6
C	-2	HIS	-	expression tag	UNP B2RKN6
C	-1	HIS	-	expression tag	UNP B2RKN6
C	0	HIS	-	expression tag	UNP B2RKN6
C	1	SER	-	expression tag	UNP B2RKN6
C	2	SER	-	expression tag	UNP B2RKN6
C	3	GLY	-	expression tag	UNP B2RKN6
C	4	VAL	-	expression tag	UNP B2RKN6
C	5	ASP	-	expression tag	UNP B2RKN6
C	6	LEU	-	expression tag	UNP B2RKN6
C	7	GLY	-	expression tag	UNP B2RKN6
C	8	THR	-	expression tag	UNP B2RKN6
C	9	GLU	-	expression tag	UNP B2RKN6
C	10	ASN	-	expression tag	UNP B2RKN6
C	11	LEU	-	expression tag	UNP B2RKN6
C	12	TYR	-	expression tag	UNP B2RKN6
C	13	PHE	-	expression tag	UNP B2RKN6
C	14	GLN	-	expression tag	UNP B2RKN6

Continued on next page...

Continued from previous page...

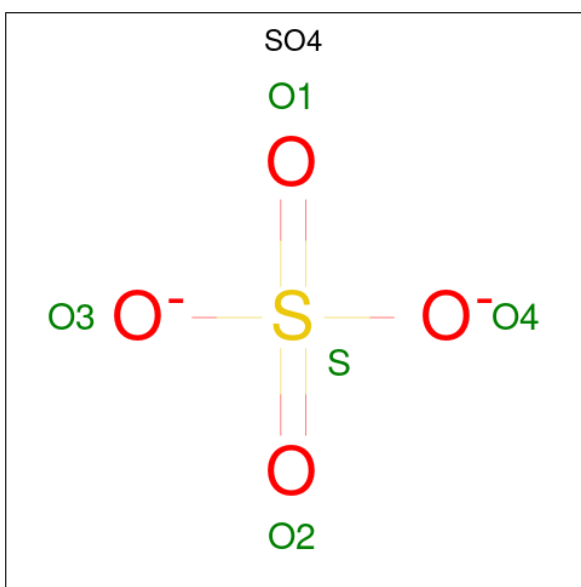
Chain	Residue	Modelled	Actual	Comment	Reference
C	15	SER	-	expression tag	UNP B2RKN6

- Molecule 2 is ADENINE (CCD ID: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	C	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

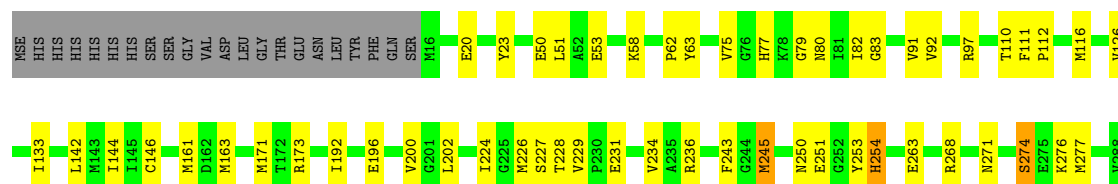
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	98	Total	O	0	0
			98	98		
4	C	97	Total	O	0	0
			97	97		

3 Residue-property plots

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

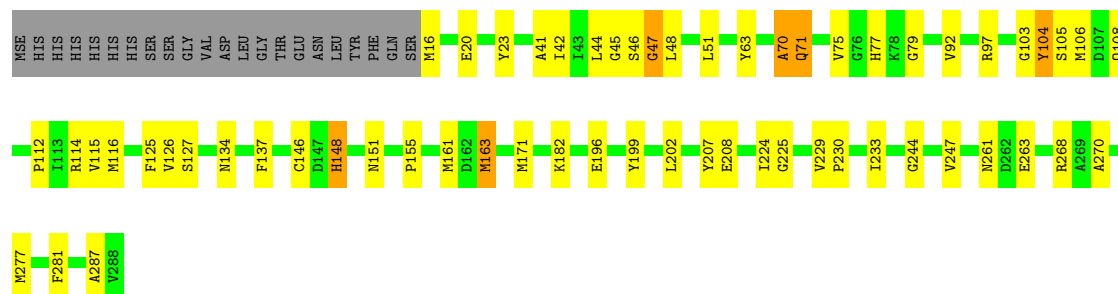
• Molecule 1: Purine nucleoside phosphorylase

Chain A: 



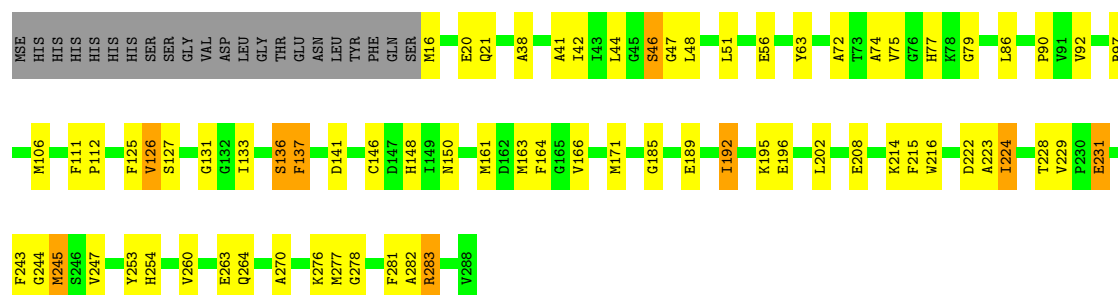
• Molecule 1: Purine nucleoside phosphorylase

Chain B: 



• Molecule 1: Purine nucleoside phosphorylase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.97Å 121.04Å 180.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.12 – 1.60 45.12 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.9 (45.12-1.60) 88.9 (45.12-1.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.193 0.170 , 0.193	Depositor DCC
R_{free} test set	4515 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	1.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.447 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.439 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.261 for H, K, L 0.383 for -1/2H+1/2K, 3/2H+1/2K, -L 0.356 for -1/2H-1/2K, -3/2H+1/2K, -L	Depositor
Outliers	0 of 90465 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6724	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CSO, SO4, ADE

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	0.69	3/2185 (0.1%)	0.93	2/2934 (0.1%)
1	B	0.83	5/2185 (0.2%)	0.97	0/2934
1	C	0.89	8/2178 (0.4%)	1.01	5/2925 (0.2%)
All	All	0.80	16/6548 (0.2%)	0.97	7/8793 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	GLN	C-O	-11.10	1.10	1.24
1	C	136[A]	SER	CA-C	10.86	1.68	1.52
1	C	136[B]	SER	CA-C	10.86	1.68	1.52
1	C	214	LYS	N-CA	9.90	1.58	1.46
1	B	70	ALA	C-O	-7.22	1.13	1.23
1	C	214	LYS	CA-C	6.61	1.61	1.52
1	A	229	VAL	C-O	-6.42	1.16	1.24
1	A	228	THR	C-O	-6.22	1.16	1.24
1	B	104	TYR	C-O	-6.10	1.16	1.23
1	C	136[A]	SER	N-CA	5.90	1.53	1.46
1	C	136[B]	SER	N-CA	5.90	1.53	1.46
1	C	74	ALA	C-O	-5.55	1.17	1.23
1	A	228	THR	CA-C	5.13	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	PHE	C-O	-5.12	1.17	1.23
1	B	103	GLY	C-O	-5.11	1.17	1.24
1	B	45	GLY	C-O	-5.01	1.19	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	LYS	CA-C-O	6.35	127.28	120.55
1	C	46	SER	N-CA-C	5.80	118.10	111.02
1	A	227	SER	N-CA-C	5.42	115.44	108.34
1	C	106	MSE	CA-CB-CG	-5.15	103.80	114.10
1	A	229	VAL	O-C-N	5.04	123.65	120.07
1	C	192	ILE	CA-C-N	-5.02	114.57	119.99
1	C	192	ILE	C-N-CA	-5.02	114.57	119.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	GLY	Peptide
1	C	136[A]	SER	Mainchain
1	C	136[B]	SER	Mainchain

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	2131	0	2138	45	0
1	B	2131	0	2138	58	0
1	C	2127	0	2125	57	0
2	A	10	0	4	0	0
2	B	10	0	4	1	0
2	C	10	0	4	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
4	A	95	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	98	0	0	14	0
4	C	97	0	0	14	0
All	All	6724	0	6413	159	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 12.

All (159) 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:B:47:GLY:CA	1:B:270:ALA:HB1	1.76	1.16
1:B:47:GLY:HA3	1:B:270:ALA:HB1	1.12	1.09
1:B:126:VAL:HB	4:B:437:HOH:O	1.51	1.08
1:C:47:GLY:HA3	1:C:270:ALA:HB3	1.33	1.07
1:B:47:GLY:CA	1:B:270:ALA:CB	2.38	1.00
1:B:47:GLY:HA2	1:B:270:ALA:HB3	1.47	0.97
1:B:47:GLY:HA2	1:B:270:ALA:CB	1.96	0.96
1:C:47:GLY:HA3	1:C:270:ALA:CB	1.96	0.93
1:B:115:VAL:HG23	4:B:482:HOH:O	1.68	0.93
1:C:202:LEU:HB3	4:C:467:HOH:O	1.70	0.91
1:B:151:ASN:HB2	4:B:465:HOH:O	1.71	0.90
1:B:171:MSE:SE	4:B:426:HOH:O	2.38	0.90
1:A:142:LEU:HD22	1:A:277:MSE:HE3	1.52	0.89
1:B:97:ARG:HD3	3:B:302:SO4:O2	1.73	0.88
1:A:58:LYS:HD2	1:A:82:ILE:HG21	1.53	0.88
1:B:233:ILE:HG23	4:B:426:HOH:O	1.75	0.86
1:B:44:LEU:HD21	1:B:51:LEU:HD12	1.61	0.81
1:B:47:GLY:HA3	1:B:270:ALA:CB	2.01	0.79
1:C:44:LEU:HD21	1:C:51:LEU:HD23	1.64	0.79
1:C:75:VAL:HB	1:C:263:GLU:OE2	1.84	0.78
1:A:50:GLU:HB3	4:A:488:HOH:O	1.84	0.78
1:A:77:HIS:HD2	1:A:97:ARG:H	1.35	0.73
1:C:146:CSO:HB2	1:C:196:GLU:OE2	1.90	0.71
1:A:75:VAL:HB	1:A:263:GLU:OE2	1.90	0.71
1:C:202:LEU:HD22	4:C:461:HOH:O	1.90	0.71
1:B:46:SER:OG	1:B:77:HIS:HE1	1.75	0.70
1:A:53:GLU:HA	4:A:424:HOH:O	1.92	0.70
1:C:282:ALA:HB2	4:C:485:HOH:O	1.91	0.69
1:C:51:LEU:HB2	4:C:447:HOH:O	1.92	0.69
1:B:23:TYR:HD1	4:B:482:HOH:O	1.75	0.68
1:B:134:ASN:HB3	1:B:137:PHE:CD1	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:HIS:HD2	1:C:97:ARG:H	1.44	0.66
1:C:21:GLN:HG2	4:C:453:HOH:O	1.95	0.66
1:C:141:ASP:OD2	1:C:195:LYS:HE3	1.94	0.66
1:B:233:ILE:HA	4:B:426:HOH:O	1.96	0.65
1:C:20:GLU:HG2	1:C:163:MSE:SE	2.46	0.65
1:B:47:GLY:CA	1:B:48:LEU:HG	2.27	0.65
1:B:42:ILE:HD11	4:B:452:HOH:O	1.96	0.64
1:C:283:ARG:HG3	4:C:493:HOH:O	1.96	0.64
1:B:281:PHE:HZ	4:B:443:HOH:O	1.80	0.63
1:C:171:MSE:SE	4:C:452:HOH:O	2.68	0.61
1:C:228:THR:O	1:C:231[A]:GLU:HG2	2.00	0.61
1:C:133:ILE:HD13	1:C:224:ILE:HG13	1.82	0.61
1:C:192:ILE:HG23	1:C:276[A]:LYS:HD3	1.83	0.60
1:A:253:TYR:O	1:A:254:HIS:ND1	2.34	0.60
1:A:200:VAL:HB	1:A:224:ILE:HG12	1.83	0.60
1:C:247:VAL:HG23	1:C:277:MSE:HE3	1.84	0.59
1:C:42:ILE:HG12	1:C:125:PHE:HB2	1.84	0.59
1:A:77:HIS:CD2	1:A:97:ARG:H	2.20	0.58
1:B:77:HIS:HD2	1:B:97:ARG:H	1.51	0.58
1:A:243:PHE:CE2	1:A:245:MSE:HG3	2.38	0.58
1:A:254:HIS:ND1	1:A:254:HIS:O	2.36	0.58
1:C:133:ILE:HD13	1:C:224:ILE:CG1	2.33	0.58
1:A:200:VAL:HG12	1:A:202:LEU:CD1	2.34	0.57
1:C:243:PHE:CE2	1:C:245:MSE:HG3	2.39	0.57
1:A:146:CSO:SG	1:A:196:GLU:HG2	2.44	0.57
1:B:281:PHE:CZ	4:B:443:HOH:O	2.52	0.57
1:C:46:SER:OG	1:C:77:HIS:HE1	1.88	0.56
1:C:86:LEU:HD11	4:C:485:HOH:O	2.04	0.56
1:A:253:TYR:CD1	1:A:254:HIS:CD2	2.94	0.56
1:C:20:GLU:HG3	1:C:161:MSE:HE1	1.87	0.56
1:A:20:GLU:HG3	1:A:161[A]:MSE:HE1	1.86	0.56
1:C:38:ALA:HA	1:C:90:PRO:HB2	1.88	0.55
1:C:253:TYR:HD1	1:C:254:HIS:HD1	1.53	0.55
1:C:245:MSE:HB3	1:C:277:MSE:HE2	1.88	0.55
1:C:77:HIS:CD2	1:C:97:ARG:H	2.23	0.55
1:A:171:MSE:SE	4:A:492:HOH:O	2.75	0.54
1:B:71:GLN:O	1:B:104:TYR:OH	2.24	0.54
1:B:47:GLY:HA3	1:B:48:LEU:HG	1.90	0.54
1:C:137:PHE:O	1:C:253:TYR:OH	2.22	0.53
1:B:20:GLU:HG3	1:B:161[A]:MSE:HE1	1.89	0.53
1:C:228:THR:HA	1:C:231[B]:GLU:OE2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:SER:OG	1:B:77:HIS:CE1	2.61	0.53
1:B:182:LYS:HB3	4:B:442:HOH:O	2.08	0.53
1:B:77:HIS:CD2	1:B:97:ARG:H	2.26	0.53
1:B:51:LEU:HB2	4:B:453:HOH:O	2.10	0.52
1:C:111:PHE:HB3	1:C:112:PRO:HD3	1.91	0.52
1:B:208:GLU:OE2	2:B:301:ADE:N1	2.42	0.52
1:A:23:TYR:HE2	1:A:161[B]:MSE:SE	2.44	0.51
1:A:23:TYR:CE2	1:A:161[B]:MSE:SE	3.13	0.51
1:B:20:GLU:HG2	1:B:163:MSE:SE	2.61	0.51
1:A:97:ARG:HH22	1:A:126:VAL:CG2	2.24	0.51
1:A:97:ARG:NH2	1:A:231:GLU:OE2	2.37	0.51
1:A:253:TYR:CE1	1:A:254:HIS:CD2	3.00	0.50
1:C:41:ALA:HA	1:C:92:VAL:O	2.11	0.50
1:C:51:LEU:O	1:C:51:LEU:HG	2.12	0.49
1:A:245:MSE:HB3	1:A:277:MSE:HE2	1.93	0.49
1:A:251:GLU:OE1	1:A:254:HIS:NE2	2.38	0.49
1:A:271:ASN:O	1:A:274:SER:OG	2.27	0.49
1:B:106:MSE:HB3	1:B:155:PRO:HA	1.95	0.49
1:B:287:ALA:HB3	4:B:442:HOH:O	2.13	0.48
1:C:166:VAL:HG22	4:C:423:HOH:O	2.14	0.48
1:A:112:PRO:O	1:A:116:MSE:HG2	2.14	0.48
1:A:144:ILE:CG1	1:A:245:MSE:HE3	2.43	0.48
1:B:146:CSO:SG	1:B:196:GLU:HG2	2.53	0.48
1:C:42:ILE:HD13	1:C:281:PHE:HD2	1.79	0.47
1:A:58:LYS:HA	1:A:83:GLY:O	2.14	0.47
1:B:112:PRO:O	1:B:116:MSE:HG2	2.15	0.47
1:C:97:ARG:HH22	1:C:126:VAL:HG23	1.80	0.47
1:B:134:ASN:HB3	1:B:137:PHE:HD1	1.77	0.46
1:C:163:MSE:HG3	1:C:164:PHE:CD2	2.50	0.46
1:B:199:TYR:OH	1:B:225:GLY:HA3	2.16	0.45
1:C:148:HIS:CG	1:C:229:VAL:HG22	2.51	0.45
1:A:110:THR:CB	1:A:234:VAL:HG21	2.47	0.45
1:B:105:SER:OG	1:B:108:GLN:HG3	2.17	0.45
1:C:185:GLY:O	1:C:189:GLU:HG3	2.16	0.45
1:B:41:ALA:HA	1:B:92:VAL:O	2.17	0.45
1:A:111:PHE:N	1:A:112:PRO:HD2	2.32	0.45
1:A:202:LEU:O	1:A:226:MSE:HA	2.17	0.45
1:B:75:VAL:HB	1:B:263:GLU:OE2	2.17	0.44
1:A:91:VAL:HG22	1:A:92:VAL:N	2.33	0.44
1:A:133:ILE:HD13	1:A:224:ILE:HG13	1.99	0.44
1:B:207:TYR:CD2	1:B:261:ASN:HB3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLY:HA3	1:C:270:ALA:HB1	1.90	0.44
1:C:215:PHE:CD1	1:C:215:PHE:C	2.94	0.44
1:A:144:ILE:HG12	1:A:245:MSE:HE3	2.00	0.43
1:C:133:ILE:HG12	1:C:222:ASP:C	2.43	0.43
1:B:77:HIS:CD2	1:B:97:ARG:HG2	2.52	0.43
1:B:229:VAL:HB	1:B:230:PRO:HD3	2.00	0.43
1:B:63:TYR:CE2	1:B:79:GLY:HA2	2.54	0.43
1:C:278:GLY:O	4:C:485:HOH:O	2.20	0.43
1:B:233:ILE:CA	4:B:426:HOH:O	2.61	0.43
1:C:126:VAL:O	1:C:244:GLY:HA2	2.19	0.43
1:B:247:VAL:HG22	1:B:277:MSE:HE3	2.01	0.42
1:B:202:LEU:CD2	1:B:224[B]:ILE:HD11	2.49	0.42
1:A:268:ARG:O	1:A:271:ASN:HB2	2.19	0.42
1:B:114:ARG:HH12	1:B:161[B]:MSE:HG3	1.85	0.42
1:C:131:GLY:O	1:C:223:ALA:HA	2.20	0.42
1:C:216:TRP:CD1	4:C:461:HOH:O	2.73	0.42
1:A:58:LYS:HD2	1:A:82:ILE:CG2	2.38	0.42
1:B:23:TYR:HE2	1:B:161[B]:MSE:SE	2.53	0.42
1:A:254:HIS:ND1	1:A:254:HIS:C	2.78	0.42
1:C:150:ASN:HB2	1:C:229:VAL:HG11	2.00	0.42
1:A:110:THR:C	1:A:112:PRO:HD2	2.44	0.42
1:A:58:LYS:NZ	4:A:424:HOH:O	2.44	0.42
1:A:192:ILE:HG12	1:A:276[A]:LYS:HD3	2.01	0.42
1:B:127:SER:HB2	1:B:277:MSE:SE	2.70	0.42
1:A:62:PRO:HA	1:A:80:ASN:OD1	2.20	0.41
1:B:171:MSE:HB3	1:B:171:MSE:HE3	1.83	0.41
1:A:236:ARG:HD2	1:A:236:ARG:HA	1.92	0.41
1:C:243:PHE:CZ	1:C:245:MSE:HG3	2.55	0.41
1:B:70:ALA:HB1	1:B:104:TYR:CE1	2.54	0.41
1:A:144:ILE:HG13	1:A:245:MSE:HE3	2.02	0.41
1:C:48:LEU:HD13	1:C:127:SER:HB2	2.02	0.41
1:C:148:HIS:CD2	1:C:148:HIS:C	2.98	0.41
1:B:125:PHE:HB3	1:B:281:PHE:CE2	2.56	0.41
1:B:148:HIS:HA	1:B:199:TYR:O	2.20	0.41
1:A:173:ARG:HH22	1:C:260:VAL:HG13	1.86	0.41
1:B:23:TYR:HE2	1:B:161[A]:MSE:HE2	1.84	0.41
1:C:56:GLU:HG2	4:C:417:HOH:O	2.20	0.41
1:C:63:TYR:CE2	1:C:79:GLY:HA2	2.56	0.41
1:C:202:LEU:CD2	4:C:461:HOH:O	2.58	0.41
1:C:208:GLU:HG2	4:C:461:HOH:O	2.22	0.40
1:A:63:TYR:CE2	1:A:79:GLY:HA2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:HD2	1:B:97:ARG:N	2.18	0.40
1:B:126:VAL:O	1:B:244:GLY:HA2	2.21	0.40
1:C:127:SER:HA	1:C:245:MSE:O	2.20	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	279/295 (95%)	272 (98%)	7 (2%)	0	100	100
1	B	279/295 (95%)	274 (98%)	5 (2%)	0	100	100
1	C	278/295 (94%)	273 (98%)	4 (1%)	1 (0%)	30	14
All	All	836/885 (94%)	819 (98%)	16 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	ALA

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	224/223 (100%)	219 (98%)	5 (2%)	45	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	224/223 (100%)	220 (98%)	4 (2%)	51	28
1	C	223/223 (100%)	215 (96%)	8 (4%)	31	10
All	All	671/669 (100%)	654 (98%)	17 (2%)	42	18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	MSE
1	A	245	MSE
1	A	250	ASN
1	A	254	HIS
1	A	274	SER
1	B	16	MSE
1	B	148	HIS
1	B	163	MSE
1	B	268	ARG
1	C	16	MSE
1	C	126	VAL
1	C	224	ILE
1	C	231[A]	GLU
1	C	231[B]	GLU
1	C	245	MSE
1	C	264	GLN
1	C	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	B	77	HIS
1	B	160	ASN
1	C	71	GLN
1	C	77	HIS
1	C	261	ASN
1	C	264	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	B	146	1	3,6,7	0.63	0	1,6,8	1.08	0
1	CSO	A	146	1	3,6,7	0.63	0	1,6,8	0.69	0
1	CSO	C	146	1	3,6,7	0.58	0	1,6,8	0.88	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
1	CSO	B	146	1	-	0/1/5/7	-
1	CSO	A	146	1	-	1/1/5/7	-
1	CSO	C	146	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	146	CSO	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	146	CSO	1	0
1	A	146	CSO	1	0
1	C	146	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	B	302	-	4,4,4	0.35	0	6,6,6	0.33	0
3	SO4	C	302	-	4,4,4	0.32	0	6,6,6	0.51	0
2	ADE	B	301	-	11,11,11	2.38	4 (36%)	15,15,15	2.51	7 (46%)
2	ADE	C	301	-	11,11,11	2.30	3 (27%)	15,15,15	2.57	6 (40%)
2	ADE	A	301	-	11,11,11	2.16	3 (27%)	15,15,15	2.93	9 (60%)
3	SO4	A	302	-	4,4,4	0.40	0	6,6,6	0.77	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
2	ADE	B	301	-	-	-	0/2/2/2
2	ADE	A	301	-	-	-	0/2/2/2
2	ADE	C	301	-	-	-	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ADE	C5-C4	6.33	1.49	1.39
2	C	301	ADE	C5-C4	5.99	1.48	1.39
2	A	301	ADE	C5-C4	5.59	1.48	1.39
2	A	301	ADE	C5-C6	3.00	1.49	1.41
2	C	301	ADE	C5-C6	2.87	1.49	1.41
2	B	301	ADE	C5-N7	-2.62	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ADE	C4-N9	-2.39	1.33	1.36
2	C	301	ADE	C5-N7	-2.34	1.34	1.39
2	B	301	ADE	C5-C6	2.28	1.47	1.41
2	A	301	ADE	C8-N7	2.12	1.36	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ADE	N9-C4-N3	5.09	134.94	126.69
2	A	301	ADE	N9-C4-N3	4.95	134.71	126.69
2	B	301	ADE	N9-C4-N3	4.83	134.51	126.69
2	A	301	ADE	N3-C2-N1	-4.64	121.55	128.58
2	B	301	ADE	C5-C4-N3	-4.48	118.59	126.75
2	C	301	ADE	C5-C4-N3	-4.38	118.76	126.75
2	A	301	ADE	C5-C4-N3	-4.16	119.17	126.75
2	A	301	ADE	C5-N7-C8	4.08	108.08	103.48
2	C	301	ADE	C5-N7-C8	3.71	107.67	103.48
2	B	301	ADE	C5-N7-C8	3.70	107.66	103.48
2	A	301	ADE	C2-N1-C6	3.62	124.68	118.73
2	C	301	ADE	N3-C2-N1	-3.46	123.35	128.58
2	B	301	ADE	C4-C5-N7	-3.35	106.02	110.67
2	A	301	ADE	C4-C5-N7	-2.96	106.56	110.67
2	A	301	ADE	C4-N9-C8	2.92	109.16	106.43
2	B	301	ADE	N3-C2-N1	-2.84	124.28	128.58
2	C	301	ADE	C4-C5-N7	-2.76	106.83	110.67
2	A	301	ADE	C6-C5-N7	2.65	137.19	132.09
2	C	301	ADE	C2-N1-C6	2.52	122.88	118.73
2	A	301	ADE	N9-C8-N7	-2.49	110.08	113.87
2	B	301	ADE	C6-C5-N7	2.26	136.44	132.09
2	B	301	ADE	C2-N1-C6	2.09	122.17	118.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	SO4	1	0
2	B	301	ADE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	261/295 (88%)	-0.91	0 100 100	9, 15, 27, 61	8 (3%)
1	B	261/295 (88%)	-0.94	0 100 100	7, 15, 26, 37	8 (3%)
1	C	261/295 (88%)	-0.94	0 100 100	7, 15, 27, 49	8 (3%)
All	All	783/885 (88%)	-0.93	0 100 100	7, 15, 26, 61	24 (3%)

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	146	7/8	0.98	0.05	12,13,18,20	0
1	CSO	B	146	7/8	0.99	0.03	12,12,21,22	0
1	CSO	C	146	7/8	0.99	0.04	12,13,21,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADE	A	301	10/10	0.97	0.07	8,8,9,9	0
2	ADE	C	301	10/10	0.98	0.04	15,18,19,20	0
2	ADE	B	301	10/10	0.99	0.02	7,8,9,9	0
3	SO4	B	302	5/5	0.99	0.05	18,18,18,23	0
3	SO4	A	302	5/5	1.00	0.03	16,17,19,19	0
3	SO4	C	302	5/5	1.00	0.03	14,15,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.