



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:06 AM GMT

PDB ID : 3KU4  
Title : Trapping of an oxocarbenium ion intermediate in UP crystals  
Authors : Paul, D.; O'Leary, S.; Rajashankar, K.; Bu, W.; Toms, A.; Settembre, E.;  
Sanders, J.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2009-11-26  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

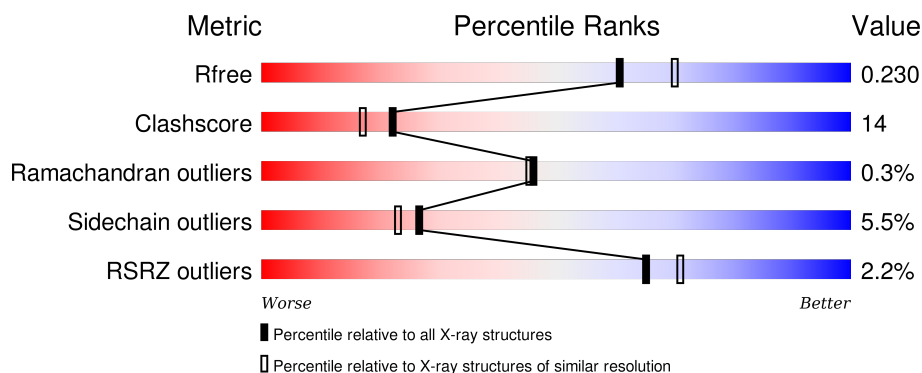
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	B	309	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	C	309	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	D	309	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9822 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2225	1408	381	414	22			
1	B	293	Total	C	N	O	S	0	0	0
			2242	1417	386	417	22			
1	C	287	Total	C	N	O	S	0	1	0
			2196	1392	373	408	23			
1	D	287	Total	C	N	O	S	0	0	0
			2185	1385	374	404	22			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

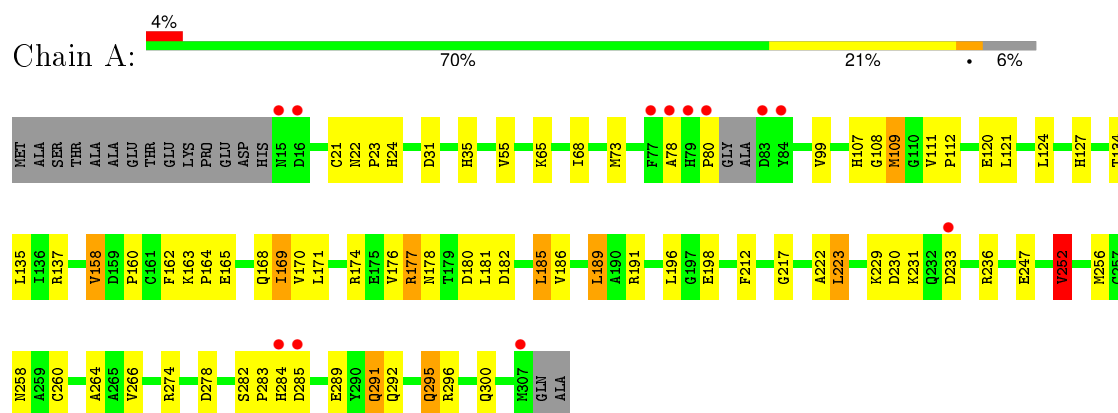
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	243	Total	O	0	0
			243	243		
3	B	264	Total	O	0	0
			264	264		
3	C	229	Total	O	0	0
			229	229		
3	D	218	Total	O	0	0
			218	218		

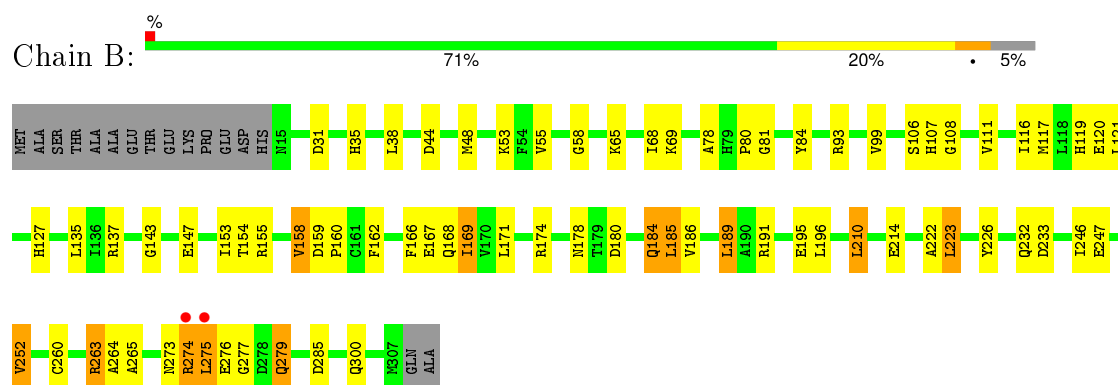
### 3 Residue-property plots [i](#)

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

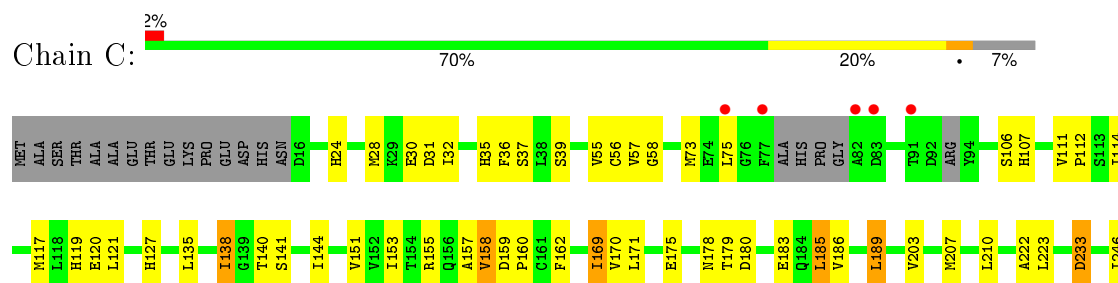
#### • Molecule 1: Uridine phosphorylase



#### • Molecule 1: Uridine phosphorylase

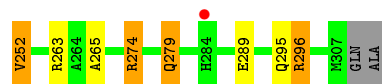
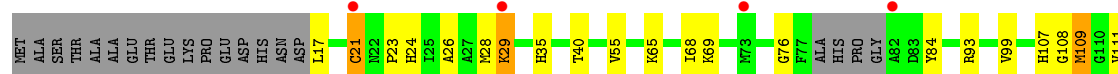


#### • Molecule 1: Uridine phosphorylase





● Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.11Å 74.11Å 266.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.10) 93.9 (49.59-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.179 , 0.225 0.187 , 0.230	Depositor DCC
$R_{free}$ test set	3904 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.7	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 78314 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	1/2265 (0.0%)	0.57	3/3060 (0.1%)
1	B	0.59	5/2286 (0.2%)	0.67	4/3093 (0.1%)
1	C	0.49	1/2239 (0.0%)	0.60	4/3025 (0.1%)
1	D	0.39	0/2226	0.56	1/3010 (0.0%)
All	All	0.49	7/9016 (0.1%)	0.60	12/12188 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	ILE	CG1-CD1	12.20	2.34	1.50
1	C	169	ILE	CG1-CD1	11.82	2.31	1.50
1	B	169	ILE	CG1-CD1	11.58	2.30	1.50
1	B	155	ARG	CZ-NH2	-10.07	1.20	1.33
1	B	155	ARG	CD-NE	-7.26	1.34	1.46
1	B	155	ARG	C-O	-6.65	1.10	1.23
1	B	155	ARG	NE-CZ	-6.30	1.24	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	80	PRO	N-CA-CB	6.05	110.56	103.30
1	C	274	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	C	169	ILE	CB-CG1-CD1	5.32	128.80	113.90
1	A	252	VAL	CB-CA-C	-5.28	101.36	111.40
1	B	233	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	285	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	233	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	285	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	285	ASP	CB-CG-OD2	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	154	THR	O-C-N	-5.09	114.56	122.70

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	2225	0	2210	74	0
1	B	2242	0	2219	72	0
1	C	2196	0	2180	61	0
1	D	2185	0	2156	62	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	243	0	0	11	1
3	B	264	0	0	6	1
3	C	229	0	0	7	1
3	D	218	0	0	5	1
All	All	9822	0	8765	244	2

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 14.

All (244) 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:D:274:ARG:HH21	1:D:274:ARG:HG2	1.16	1.11
1:B:169:ILE:CD1	1:B:169:ILE:CG1	2.30	1.09
1:C:169:ILE:CD1	1:C:169:ILE:CG1	2.32	1.08
1:A:68:ILE:HD11	1:A:99:VAL:HG12	1.28	1.08
1:A:169:ILE:CD1	1:A:169:ILE:CG1	2.34	1.05
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.16	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ARG:HH11	1:D:296:ARG:HB3	1.22	1.00
1:B:222:ALA:C	1:B:223:LEU:HD13	1.80	1.00
1:A:212:PHE:HB3	1:B:116:ILE:HD11	1.42	0.99
1:A:222:ALA:C	1:A:223:LEU:HD12	1.83	0.98
1:D:274:ARG:HG2	1:D:274:ARG:NH2	1.76	0.94
1:A:260:CYS:SG	1:B:223:LEU:HD11	2.08	0.93
1:A:68:ILE:CD1	1:A:99:VAL:HG12	1.99	0.91
1:D:274:ARG:HH21	1:D:274:ARG:CG	1.83	0.91
1:A:191:ARG:HB3	3:A:865:HOH:O	1.71	0.89
1:A:233:ASP:OD1	1:A:236:ARG:NH2	2.05	0.89
1:C:274:ARG:HD2	1:C:278:ASP:OD1	1.76	0.86
1:A:21:CYS:HB2	1:B:223:LEU:HD12	1.57	0.85
1:C:119:HIS:HD2	1:D:222:ALA:H	1.27	0.82
1:B:222:ALA:O	1:B:223:LEU:HD13	1.81	0.81
1:A:160:PRO:HB2	1:B:169:ILE:HG21	1.62	0.81
1:C:112:PRO:HB2	1:D:109:MET:HE1	1.64	0.79
1:B:31:ASP:OD2	1:B:127:HIS:HE1	1.63	0.79
1:C:284:HIS:HD2	3:C:593:HOH:O	1.65	0.79
1:D:246:ILE:HD12	1:D:274:ARG:HE	1.48	0.78
1:D:296:ARG:NH1	1:D:296:ARG:HB3	1.99	0.77
1:B:274:ARG:O	1:B:277:GLY:N	2.17	0.77
1:C:185:LEU:HD13	1:C:265:ALA:HB2	1.67	0.76
1:A:35:HIS:HD2	1:A:120:GLU:OE2	1.69	0.76
1:A:177:ARG:CG	1:A:177:ARG:HH11	1.97	0.76
1:A:109:MET:HG2	1:B:93:ARG:CZ	2.17	0.75
1:C:56:CYS:SG	1:C:138:ILE:HD12	2.27	0.75
1:C:112:PRO:HB2	1:D:109:MET:CE	2.17	0.74
1:B:279:GLN:H	1:B:279:GLN:NE2	1.86	0.73
1:C:140:THR:HG23	1:C:271:LEU:HG	1.69	0.73
1:C:222:ALA:H	1:D:119:HIS:HD2	1.36	0.73
1:A:111:VAL:HG22	1:A:252:VAL:HG22	1.71	0.72
1:A:222:ALA:H	1:B:119:HIS:HD2	1.36	0.72
1:C:31:ASP:OD2	1:C:127:HIS:HE1	1.71	0.72
1:C:35:HIS:HD2	1:C:120:GLU:OE2	1.71	0.72
3:C:321:HOH:O	1:D:119:HIS:HE1	1.72	0.71
1:C:274:ARG:HD3	3:C:918:HOH:O	1.89	0.71
1:D:111:VAL:HG22	1:D:252:VAL:HG22	1.71	0.71
1:D:24:HIS:O	1:D:28:MET:HG3	1.91	0.71
1:C:170:VAL:O	1:C:171:LEU:HB2	1.89	0.71
1:D:35:HIS:HD2	1:D:120:GLU:OE2	1.74	0.71
1:A:170:VAL:O	1:A:171:LEU:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:O	1:A:229:LYS:HD3	1.92	0.70
1:A:112:PRO:HG3	1:B:210:LEU:HD22	1.72	0.70
1:A:212:PHE:CB	1:B:116:ILE:HD11	2.19	0.70
1:A:256:MET:HE2	3:A:952:HOH:O	1.91	0.70
1:B:246:ILE:HD12	1:B:274:ARG:CD	2.22	0.70
1:D:29:LYS:NZ	1:D:29:LYS:HB2	2.06	0.70
1:C:138:ILE:HD13	1:C:138:ILE:H	1.56	0.70
1:A:178:ASN:ND2	1:A:180:ASP:H	1.88	0.69
1:C:178:ASN:HD21	1:C:180:ASP:HB2	1.58	0.69
1:D:232:GLN:O	1:D:236:ARG:HG2	1.93	0.69
1:A:177:ARG:NH1	1:A:177:ARG:HG3	1.96	0.68
1:A:223:LEU:HD12	1:A:223:LEU:N	2.08	0.68
1:D:216:GLN:O	1:D:274:ARG:NH1	2.27	0.68
1:D:216:GLN:HB3	1:D:274:ARG:NH1	2.08	0.67
1:A:185:LEU:HD22	1:A:189:LEU:HD22	1.76	0.67
1:D:161:CYS:HB2	1:D:163:LYS:HD3	1.77	0.67
1:C:233:ASP:OD1	3:C:316:HOH:O	2.13	0.66
1:A:169:ILE:HD12	3:A:388:HOH:O	1.96	0.66
1:A:55:VAL:HG11	1:A:121:LEU:HD21	1.78	0.66
1:C:260:CYS:SG	1:D:223:LEU:HD21	2.36	0.65
1:C:119:HIS:CD2	1:D:222:ALA:H	2.14	0.65
1:B:273:ASN:O	1:B:275:LEU:N	2.30	0.65
1:B:55:VAL:HG13	3:B:402:HOH:O	1.97	0.65
1:B:147:GLU:HG2	3:B:339:HOH:O	1.97	0.64
1:B:167:GLU:OE1	1:B:174:ARG:HD3	2.00	0.62
1:D:159:ASP:HB3	1:D:161:CYS:H	1.63	0.62
1:C:57:VAL:O	1:C:138:ILE:HD13	2.00	0.61
1:B:44:ASP:O	1:B:48:MET:HG3	2.00	0.61
1:D:107:HIS:HE1	1:D:137:ARG:HH11	1.49	0.61
1:B:107:HIS:HB3	1:B:117:MET:CE	2.31	0.60
1:C:119:HIS:HD2	1:D:222:ALA:N	1.98	0.60
1:C:55:VAL:HG11	1:C:121:LEU:HD21	1.82	0.60
1:A:223:LEU:N	1:A:223:LEU:CD1	2.63	0.60
1:B:158:VAL:HG13	1:B:162:PHE:HA	1.84	0.60
1:A:107:HIS:HD2	1:A:108:GLY:O	1.85	0.60
1:B:274:ARG:O	1:B:275:LEU:C	2.39	0.59
1:C:24:HIS:O	1:C:28:MET:HG3	2.02	0.59
1:A:31:ASP:OD2	1:A:127:HIS:HE1	1.85	0.59
1:D:111:VAL:HG22	1:D:252:VAL:CG2	2.33	0.59
1:D:107:HIS:HD2	1:D:108:GLY:O	1.85	0.59
1:B:223:LEU:N	1:B:223:LEU:HD13	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:HIS:HD2	3:C:503:HOH:O	1.84	0.59
1:B:78:ALA:HB3	3:B:754:HOH:O	2.03	0.59
1:B:107:HIS:HB3	1:B:117:MET:HE3	1.84	0.58
1:A:169:ILE:CD1	3:A:388:HOH:O	2.50	0.58
3:A:314:HOH:O	1:B:119:HIS:HE1	1.87	0.58
1:B:185:LEU:HD13	1:B:265:ALA:HB2	1.86	0.58
1:B:55:VAL:HG11	1:B:121:LEU:HD21	1.85	0.58
1:D:185:LEU:HD13	1:D:265:ALA:HB2	1.86	0.57
1:C:107:HIS:CG	1:C:114:ILE:HD13	2.39	0.57
1:D:296:ARG:HH11	1:D:296:ARG:CB	2.08	0.57
1:C:222:ALA:C	1:C:223:LEU:HD12	2.26	0.56
1:C:111:VAL:HG22	1:C:252:VAL:CG2	2.35	0.56
1:C:140:THR:CG2	1:C:141:SER:N	2.69	0.56
1:A:284:HIS:HB2	3:A:350:HOH:O	2.05	0.56
1:B:274:ARG:O	1:B:277:GLY:O	2.24	0.56
1:A:256:MET:CE	3:A:952:HOH:O	2.50	0.56
1:B:273:ASN:O	1:B:274:ARG:C	2.43	0.56
1:D:143:GLY:O	1:D:144:ILE:HD13	2.05	0.55
1:C:111:VAL:HG13	1:C:252:VAL:HG21	1.88	0.55
1:B:246:ILE:HD12	1:B:274:ARG:NE	2.22	0.55
1:C:140:THR:HG22	1:C:141:SER:N	2.22	0.55
1:C:107:HIS:HB3	1:C:117:MET:CE	2.37	0.55
1:D:166:PHE:CZ	1:D:252:VAL:HG13	2.42	0.54
1:B:166:PHE:CZ	1:B:252:VAL:HG13	2.42	0.54
1:A:134:THR:HG23	1:A:185:LEU:HD11	1.88	0.54
1:A:274:ARG:NH2	1:A:278:ASP:OD1	2.40	0.54
1:B:275:LEU:C	1:B:277:GLY:H	2.11	0.54
1:B:107:HIS:HD2	1:B:108:GLY:O	1.91	0.54
1:A:191:ARG:HD2	3:A:865:HOH:O	2.07	0.54
1:C:107:HIS:HB3	1:C:117:MET:HE2	1.90	0.54
1:A:65:LYS:O	1:A:68:ILE:HG22	2.08	0.54
1:A:222:ALA:O	1:A:223:LEU:HD12	2.07	0.54
1:D:76:GLY:HA2	3:D:665:HOH:O	2.07	0.54
1:B:107:HIS:HE1	1:B:137:ARG:HH11	1.57	0.53
1:B:35:HIS:HD2	1:B:120:GLU:OE2	1.91	0.53
1:D:279:GLN:H	1:D:279:GLN:NE2	2.06	0.53
1:D:55:VAL:HG11	1:D:121:LEU:HD21	1.90	0.52
1:D:166:PHE:HD1	3:D:354:HOH:O	1.92	0.52
1:A:196:LEU:HD21	1:A:300:GLN:HG3	1.91	0.52
1:B:153:ILE:HD13	1:B:189:LEU:HB3	1.91	0.52
1:B:222:ALA:O	1:B:223:LEU:CD1	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:N	3:D:735:HOH:O	2.42	0.52
1:B:178:ASN:ND2	1:B:180:ASP:H	2.07	0.51
1:A:295:GLN:NE2	3:A:490:HOH:O	2.43	0.51
1:D:158:VAL:HG22	1:D:206:THR:O	2.10	0.51
1:C:107:HIS:CB	1:C:114:ILE:HD13	2.40	0.51
1:A:222:ALA:H	1:B:119:HIS:CD2	2.24	0.51
1:C:58:GLY:O	1:C:106:SER:HA	2.11	0.51
1:C:140:THR:CG2	1:C:271:LEU:HG	2.38	0.50
1:A:222:ALA:N	1:B:119:HIS:HD2	2.05	0.50
1:A:181:LEU:HD21	1:A:266:VAL:HG23	1.93	0.50
1:C:112:PRO:CB	1:D:109:MET:HE1	2.39	0.50
1:A:158:VAL:CG1	1:A:162:PHE:HA	2.42	0.50
1:B:275:LEU:O	1:B:277:GLY:N	2.45	0.49
1:C:111:VAL:HB	1:C:112:PRO:HD3	1.93	0.49
1:A:168:GLN:NE2	1:B:214:GLU:OE2	2.44	0.49
1:D:246:ILE:CD1	1:D:274:ARG:HE	2.21	0.49
1:D:144:ILE:HD13	1:D:274:ARG:HB2	1.94	0.49
1:C:223:LEU:N	1:C:223:LEU:HD12	2.27	0.49
1:C:303:LYS:O	1:C:307:MET:SD	2.71	0.49
1:A:177:ARG:CG	1:A:177:ARG:NH1	2.65	0.49
1:A:111:VAL:HG22	1:A:252:VAL:CG2	2.40	0.48
1:B:65:LYS:HE2	1:B:69:LYS:HE3	1.95	0.48
1:B:184:GLN:CG	1:B:263:ARG:HH22	2.26	0.48
1:B:159:ASP:HB2	1:B:160:PRO:CD	2.44	0.48
1:D:178:ASN:ND2	1:D:180:ASP:H	2.12	0.48
1:D:274:ARG:NH2	1:D:274:ARG:CG	2.50	0.48
1:A:170:VAL:O	1:A:171:LEU:CB	2.59	0.48
1:D:211:ASP:OD2	1:D:214:GLU:HB2	2.13	0.48
1:C:274:ARG:CD	1:C:278:ASP:OD1	2.55	0.47
1:D:26:ALA:HB3	3:D:459:HOH:O	2.14	0.47
1:C:222:ALA:N	1:D:119:HIS:HD2	2.09	0.47
1:D:235:LEU:HD13	1:D:274:ARG:HB3	1.96	0.47
1:A:178:ASN:HD21	1:A:180:ASP:CB	2.27	0.47
1:C:207:MET:HB3	1:C:246:ILE:CD1	2.45	0.47
1:C:32:ILE:HD13	1:C:39:SER:HB2	1.96	0.47
1:A:217:GLY:O	1:A:231:LYS:HD3	2.14	0.47
1:A:107:HIS:HE1	1:A:137:ARG:HH11	1.63	0.47
1:B:111:VAL:HG22	1:B:252:VAL:HG22	1.96	0.46
1:D:21:CYS:O	1:D:23:PRO:HD3	2.15	0.46
1:C:73:MET:HG2	3:C:443:HOH:O	2.15	0.46
1:C:151:VAL:HG21	3:C:749:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LYS:HB2	1:D:29:LYS:HZ3	1.79	0.46
1:D:107:HIS:CE1	1:D:137:ARG:HH11	2.32	0.46
1:A:24:HIS:HE1	1:B:226:TYR:O	1.98	0.46
1:D:69:LYS:HG2	1:D:84:TYR:CE2	2.50	0.46
1:A:158:VAL:HG13	1:A:162:PHE:HA	1.98	0.46
1:C:144:ILE:HD11	1:C:246:ILE:HD11	1.98	0.46
1:B:53:LYS:HD2	3:B:326:HOH:O	2.16	0.46
1:B:158:VAL:CG1	1:B:162:PHE:HA	2.45	0.46
1:A:222:ALA:C	1:A:223:LEU:CD1	2.71	0.46
1:B:232:GLN:NE2	1:B:275:LEU:O	2.49	0.45
1:D:279:GLN:H	1:D:279:GLN:CD	2.20	0.45
1:D:29:LYS:HB2	1:D:29:LYS:HZ2	1.78	0.45
1:C:36:PHE:O	1:C:37:SER:HB2	2.16	0.45
1:A:178:ASN:HD21	1:A:180:ASP:H	1.60	0.45
1:A:182:ASP:OD1	1:A:185:LEU:HB2	2.16	0.45
1:B:279:GLN:H	1:B:279:GLN:HE21	1.61	0.45
1:A:135:LEU:O	1:A:264:ALA:HA	2.18	0.44
1:D:68:ILE:HD11	1:D:99:VAL:HG12	1.98	0.44
1:B:275:LEU:C	1:B:277:GLY:N	2.70	0.44
1:C:140:THR:HG21	1:C:271:LEU:CD1	2.47	0.44
1:C:210:LEU:CD2	1:D:210:LEU:HD11	2.48	0.44
1:A:292:GLN:HG3	3:A:352:HOH:O	2.16	0.44
1:C:178:ASN:ND2	1:C:180:ASP:H	2.16	0.44
1:A:163:LYS:HA	1:A:164:PRO:HD3	1.83	0.44
1:C:159:ASP:HB2	1:C:160:PRO:CD	2.48	0.44
1:B:273:ASN:OD1	1:B:273:ASN:O	2.36	0.43
1:B:68:ILE:HD11	1:B:99:VAL:HG12	1.99	0.43
1:C:30:GLU:OE2	1:C:32:ILE:HD11	2.19	0.43
1:A:73:MET:HA	1:A:78:ALA:HB2	2.00	0.43
1:B:107:HIS:HB3	1:B:117:MET:HE2	2.00	0.43
1:A:284:HIS:CD2	3:A:739:HOH:O	2.71	0.43
1:A:291:GLN:HB2	1:A:291:GLN:HE21	1.47	0.43
1:B:196:LEU:HD21	1:B:300:GLN:HG3	2.00	0.43
1:D:93:ARG:HD2	3:D:700:HOH:O	2.18	0.43
1:D:156:GLN:HG2	1:D:180:ASP:OD1	2.19	0.43
1:C:157:ALA:HB3	1:C:179:THR:HB	2.01	0.43
1:B:246:ILE:HD12	1:B:274:ARG:HD2	1.99	0.42
1:B:84:TYR:N	1:B:84:TYR:CD2	2.86	0.42
1:B:143:GLY:O	1:B:274:ARG:HG3	2.19	0.42
1:C:55:VAL:HB	1:C:135:LEU:HG	1.99	0.42
1:C:207:MET:CE	1:C:246:ILE:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:PHE:CD2	1:D:162:PHE:N	2.84	0.42
1:A:282:SER:HA	1:A:283:PRO:HD3	1.83	0.42
1:D:170:VAL:O	1:D:171:LEU:HB2	2.18	0.42
1:D:159:ASP:HB2	1:D:163:LYS:H	1.83	0.42
1:B:159:ASP:HB2	1:B:160:PRO:HD2	2.01	0.42
1:B:80:PRO:HA	1:B:81:GLY:HA2	1.71	0.42
1:C:153:ILE:HD13	1:C:189:LEU:HB3	2.02	0.42
1:A:165:GLU:HB3	1:A:176:VAL:HG13	2.02	0.42
1:A:198:GLU:OE1	1:A:296:ARG:NH1	2.53	0.42
1:A:124:LEU:HD23	1:A:124:LEU:C	2.40	0.42
1:A:212:PHE:CD1	1:B:116:ILE:HD11	2.55	0.42
1:C:289:GLU:OE1	1:C:296:ARG:NH2	2.48	0.42
1:A:22:ASN:HA	1:A:23:PRO:HD2	1.91	0.42
1:B:55:VAL:CG1	3:B:402:HOH:O	2.59	0.42
1:C:135:LEU:O	1:C:264:ALA:HA	2.20	0.42
1:A:258:ASN:HD22	1:A:258:ASN:HA	1.60	0.42
1:B:35:HIS:HE1	3:B:898:HOH:O	2.02	0.41
1:A:230:ASP:HB3	1:B:171:LEU:HD11	2.02	0.41
1:B:58:GLY:O	1:B:106:SER:HA	2.21	0.41
1:D:65:LYS:O	1:D:68:ILE:HG22	2.20	0.41
1:C:75:LEU:HA	1:C:75:LEU:HD23	1.88	0.41
1:A:181:LEU:CD2	1:A:266:VAL:HG23	2.50	0.41
1:C:158:VAL:HG13	1:C:162:PHE:HA	2.03	0.41
1:A:223:LEU:HD11	1:B:260:CYS:SG	2.61	0.41
1:D:55:VAL:HB	1:D:135:LEU:HG	2.03	0.41
1:D:246:ILE:HD12	1:D:274:ARG:NE	2.27	0.41
1:A:162:PHE:N	1:A:162:PHE:CD2	2.86	0.41
1:B:99:VAL:O	1:B:99:VAL:HG13	2.22	0.40
1:D:182:ASP:OD2	1:D:263:ARG:HD2	2.21	0.40
1:A:178:ASN:HD21	1:A:180:ASP:CG	2.25	0.40
1:C:155:ARG:NH1	1:C:183:GLU:OE2	2.54	0.40
1:B:135:LEU:O	1:B:264:ALA:HA	2.21	0.40
1:B:191:ARG:O	1:B:195:GLU:HG3	2.22	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
3:C:358:HOH:O	3:D:357:HOH:O[4_564]	2.09	0.11
3:A:376:HOH:O	3:B:375:HOH:O[4_554]	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	287/309 (93%)	283 (99%)	4 (1%)	0	100	100
1	B	291/309 (94%)	282 (97%)	6 (2%)	3 (1%)	19	13
1	C	282/309 (91%)	275 (98%)	7 (2%)	0	100	100
1	D	283/309 (92%)	281 (99%)	2 (1%)	0	100	100
All	All	1143/1236 (92%)	1121 (98%)	19 (2%)	3 (0%)	46	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	274	ARG
1	B	275	LEU
1	B	276	GLU

### 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	239/255 (94%)	226 (95%)	13 (5%)	27	24
1	B	241/255 (94%)	228 (95%)	13 (5%)	27	24
1	C	237/255 (93%)	228 (96%)	9 (4%)	40	40
1	D	232/255 (91%)	215 (93%)	17 (7%)	17	13
All	All	949/1020 (93%)	897 (94%)	52 (6%)	27	23

All (52) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	109	MET
1	A	158	VAL
1	A	174	ARG
1	A	177	ARG
1	A	185	LEU
1	A	186	VAL
1	A	189	LEU
1	A	223	LEU
1	A	247	GLU
1	A	252	VAL
1	A	289	GLU
1	A	291	GLN
1	A	295	GLN
1	B	38	LEU
1	B	158	VAL
1	B	168	GLN
1	B	184	GLN
1	B	185	LEU
1	B	186	VAL
1	B	189	LEU
1	B	210	LEU
1	B	223	LEU
1	B	247	GLU
1	B	252	VAL
1	B	263	ARG
1	B	279	GLN
1	C	138	ILE
1	C	158	VAL
1	C	175	GLU
1	C	185	LEU
1	C	186	VAL
1	C	189	LEU
1	C	203	VAL
1	C	247	GLU
1	C	307	MET
1	D	21	CYS
1	D	29	LYS
1	D	40	THR
1	D	109	MET
1	D	155	ARG
1	D	162	PHE
1	D	163	LYS
1	D	185	LEU

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Mol	Chain	Res	Type
1	D	186	VAL
1	D	203	VAL
1	D	247	GLU
1	D	252	VAL
1	D	274	ARG
1	D	279	GLN
1	D	289	GLU
1	D	295	GLN
1	D	296	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	35	HIS
1	A	107	HIS
1	A	127	HIS
1	A	178	ASN
1	A	258	ASN
1	A	291	GLN
1	A	295	GLN
1	B	35	HIS
1	B	107	HIS
1	B	119	HIS
1	B	127	HIS
1	B	168	GLN
1	B	178	ASN
1	B	184	GLN
1	B	279	GLN
1	C	35	HIS
1	C	119	HIS
1	C	127	HIS
1	C	178	ASN
1	C	284	HIS
1	C	295	GLN
1	D	35	HIS
1	D	107	HIS
1	D	119	HIS
1	D	178	ASN
1	D	187	GLN
1	D	279	GLN
1	D	295	GLN

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Mol	Chain	Res	Type
1	D	300	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](#)

4 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	$\# Z  > 2$
2	SO4	A	310	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	B	310	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	C	310	-	4,4,4	0.18	0	6,6,6	0.21	0
2	SO4	D	310	-	4,4,4	0.21	0	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	310	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	310	-	-	0/0/0/0	0/0/0/0
2	SO4	C	310	-	-	0/0/0/0	0/0/0/0
2	SO4	D	310	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	291/309 (94%)	0.01	12 (4%) 41 50	15, 23, 41, 64	0
1	B	293/309 (94%)	-0.01	2 (0%) 89 91	14, 21, 38, 54	0
1	C	287/309 (92%)	-0.11	6 (2%) 67 72	14, 21, 39, 56	0
1	D	287/309 (92%)	-0.12	6 (2%) 67 72	14, 23, 39, 51	0
All	All	1158/1236 (93%)	-0.06	26 (2%) 65 71	14, 22, 39, 64	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	PRO	9.0
1	B	274	ARG	6.0
1	A	78	ALA	5.4
1	A	79	HIS	4.2
1	C	307	MET	4.1
1	B	275	LEU	3.7
1	A	15	ASN	3.7
1	A	285	ASP	3.5
1	C	82	ALA	3.2
1	D	21	CYS	3.2
1	C	83	ASP	3.1
1	A	284	HIS	3.1
1	D	82	ALA	3.0
1	A	233	ASP	2.9
1	C	77	PHE	2.7
1	A	83	ASP	2.7
1	C	75	LEU	2.6
1	D	29	LYS	2.5
1	D	73	MET	2.5
1	A	84	TYR	2.5
1	A	16	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	PHE	2.4
1	D	284	HIS	2.3
1	D	169	ILE	2.2
1	C	91	THR	2.1
1	A	307	MET	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	310	5/5	0.99	0.09	-2.71	18,22,24,26	0
2	SO4	A	310	5/5	0.91	0.16	-	31,37,48,52	0
2	SO4	D	310	5/5	0.98	0.08	-	25,26,31,31	0
2	SO4	C	310	5/5	0.99	0.07	-	25,26,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.