



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:38 pm GMT

PDB ID : 3K56  
Title : Crystal Structure of Isopentenyl Phosphate Kinase from *M. jannaschii* in complex with IPP beta-S  
Authors : Dellas, N.; Noel, J.P.  
Deposited on : 2009-10-06  
Resolution : 2.34 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 : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

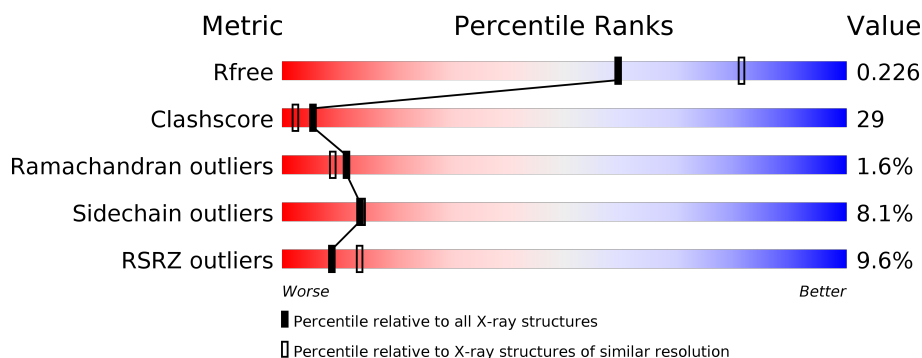
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	266	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>34%</div> <div>• •</div> </div> </div>
1	B	266	<div> <div>14%</div> <div> <div></div> <div>48%</div> <div>37%</div> <div>8%</div> <div>• 7%</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
2	IS3	A	300	-	-	X	-
3	SO4	A	303	-	-	X	-
3	SO4	B	301	-	-	-	X
3	SO4	B	302	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4205 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.

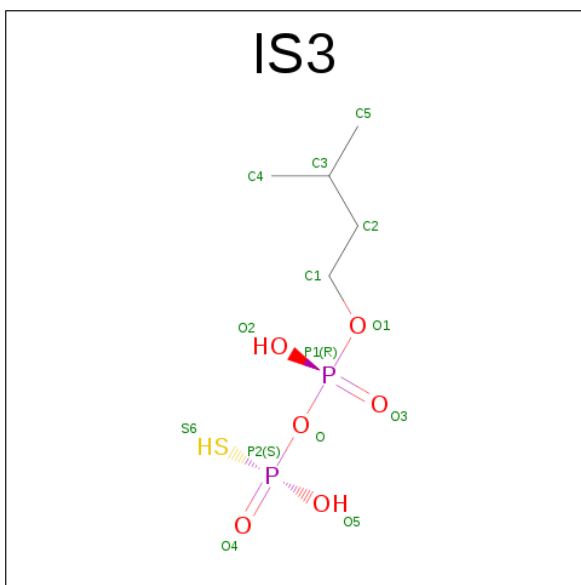
- Molecule 1 is a protein called isopentenyl phosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	3	0
			2090	1345	351	386	8			
1	B	248	Total	C	N	O	S	0	0	0
			1999	1295	335	361	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q60352
A	-4	SER	-	EXPRESSION TAG	UNP Q60352
A	-3	HIS	-	EXPRESSION TAG	UNP Q60352
A	-2	GLY	-	EXPRESSION TAG	UNP Q60352
A	-1	GLY	-	EXPRESSION TAG	UNP Q60352
A	0	SER	-	EXPRESSION TAG	UNP Q60352
A	223	GLU	ASP	CONFLICT	UNP Q60352
B	-5	GLY	-	EXPRESSION TAG	UNP Q60352
B	-4	SER	-	EXPRESSION TAG	UNP Q60352
B	-3	HIS	-	EXPRESSION TAG	UNP Q60352
B	-2	GLY	-	EXPRESSION TAG	UNP Q60352
B	-1	GLY	-	EXPRESSION TAG	UNP Q60352
B	0	SER	-	EXPRESSION TAG	UNP Q60352
B	223	GLU	ASP	CONFLICT	UNP Q60352

- Molecule 2 is ISOPENTENYL DIPHOSPHATE BETA-S (three-letter code: IS3) (formula: C<sub>5</sub>H<sub>14</sub>O<sub>6</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			14	5	6	2	1		
2	B	1	Total	C	O	P	S	0	0
			14	5	6	2	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	A	1	Total	O	S	0	0
			5	4	1		

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

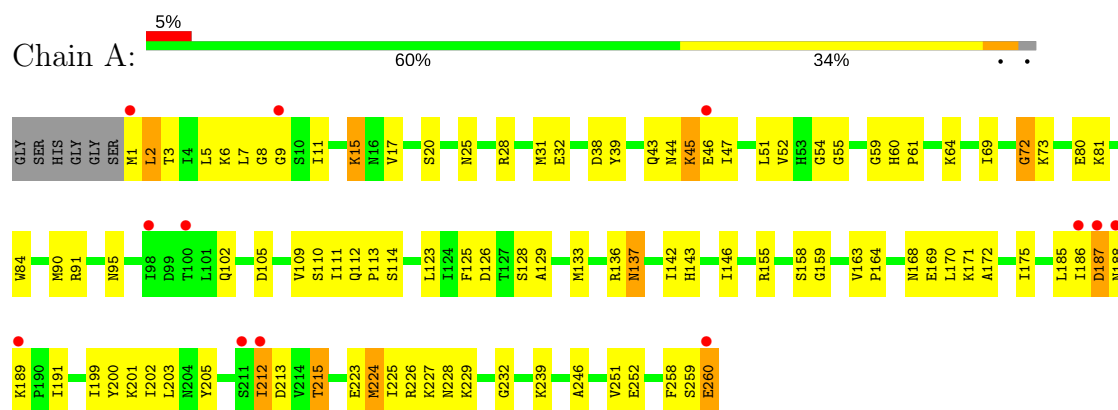
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	27	Total	O	0	0
			27	27		

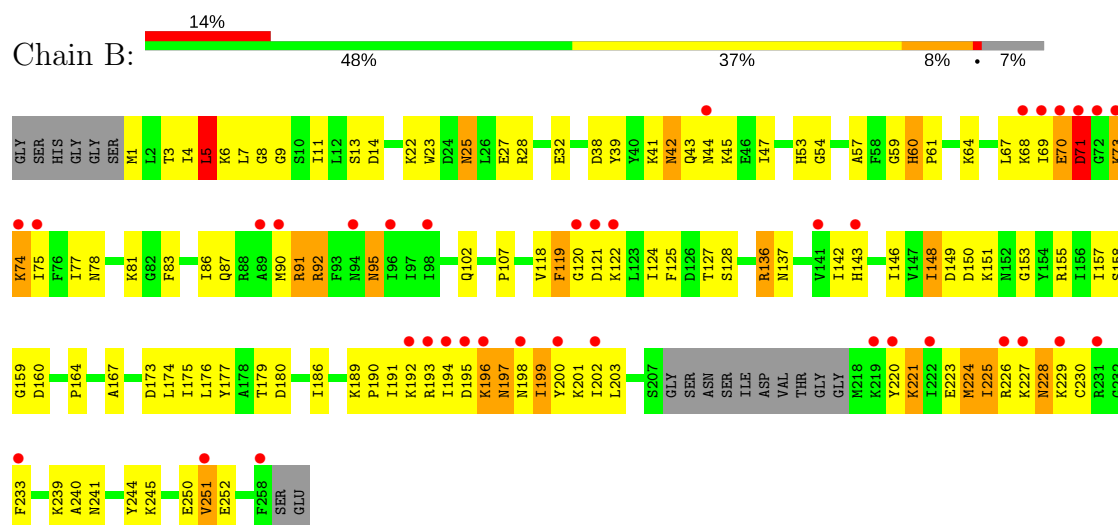
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: isopentenyl phosphate kinase



#### • Molecule 1: isopentenyl phosphate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.68Å 100.24Å 87.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.11 – 2.34 42.11 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.11-2.34) 99.4 (42.11-2.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.220 , 0.259 0.221 , 0.226	Depositor DCC
$R_{free}$ test set	1485 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IS3, 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	0.96	0/2125	0.95	1/2858 (0.0%)
1	B	0.91	0/2033	0.98	5/2733 (0.2%)
All	All	0.94	0/4158	0.97	6/5591 (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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	71	ASP	N-CA-C	8.14	132.99	111.00
1	B	136	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	224	MET	CG-SD-CE	6.65	110.84	100.20
1	B	91	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	60	HIS	C-N-CD	5.11	139.12	128.40
1	B	5	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	GLU	Peptide
1	B	71	ASP	Peptide

## 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	2090	0	2154	122	0
1	B	1999	0	2076	132	0
2	A	14	0	11	6	0
2	B	14	0	11	5	0
3	A	10	0	0	5	0
3	B	10	0	0	2	0
4	A	41	0	0	2	0
4	B	27	0	0	4	0
All	All	4205	0	4252	241	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 29.

All (241) 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:74:LYS:O	1:B:75:ILE:HD13	1.28	1.30
1:A:72:GLY:O	1:A:73:LYS:HG2	1.45	1.17
1:A:260:GLU:HA	1:A:260:GLU:OE2	1.42	1.11
1:A:212:ILE:HD12	1:A:212:ILE:H	1.15	1.09
1:B:90:MET:HA	1:B:90:MET:HE2	1.28	1.07
1:A:9[B]:GLY:HA2	3:A:303:SO4:O3	1.58	1.02
1:B:1:MET:N	1:B:173:ASP:OD2	1.92	1.01
1:A:91:ARG:HH11	1:A:112:GLN:HE22	1.07	1.01
1:A:45:LYS:HE3	1:A:46:GLU:H	1.25	1.01
1:B:199:ILE:HD11	1:B:203:LEU:HD21	1.43	1.01
1:A:260:GLU:OE2	1:A:260:GLU:CA	2.15	0.95
1:A:110:SER:H	1:B:87:GLN:HE22	1.16	0.90
1:B:74:LYS:C	1:B:75:ILE:HD13	1.93	0.89
1:A:199:ILE:HD13	1:A:226:ARG:HE	1.39	0.87
1:B:90:MET:CE	1:B:90:MET:HA	2.03	0.87
1:B:90:MET:CA	1:B:90:MET:HE2	2.03	0.87
1:B:240:ALA:O	1:B:241:ASN:HB2	1.75	0.86
1:A:69:ILE:HA	1:A:73:LYS:O	1.75	0.86
1:A:45:LYS:HE3	1:A:46:GLU:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HE	1:B:95:ASN:HD21	1.25	0.83
1:A:72:GLY:O	1:A:73:LYS:CG	2.28	0.82
1:A:163:VAL:HB	1:A:164:PRO:HD3	1.60	0.82
1:A:251:VAL:HG22	1:A:252:GLU:N	1.92	0.82
1:B:199:ILE:HG12	1:B:203:LEU:HD22	1.61	0.81
1:A:9[B]:GLY:CA	3:A:303:SO4:O3	2.28	0.81
1:B:167:ALA:HB1	1:B:175:ILE:HD11	1.63	0.80
1:A:7:LEU:O	1:A:8[B]:GLY:C	2.18	0.80
1:A:105:ASP:OD1	1:B:81:LYS:NZ	2.15	0.78
1:B:159:GLY:N	2:B:300:IS3:O2	2.14	0.78
1:B:74:LYS:O	1:B:75:ILE:CD1	2.22	0.77
1:B:90:MET:CA	1:B:90:MET:CE	2.63	0.76
1:B:54:GLY:HA3	2:B:300:IS3:O	1.85	0.76
1:A:212:ILE:CD1	1:A:212:ILE:H	1.93	0.75
1:A:163:VAL:HB	1:A:164:PRO:CD	2.16	0.75
1:B:199:ILE:CD1	1:B:203:LEU:HD21	2.15	0.75
1:A:6:LYS:HE3	3:A:303:SO4:O4	1.87	0.74
1:B:199:ILE:CD1	1:B:203:LEU:CD2	2.65	0.74
1:A:69:ILE:HG23	1:A:73:LYS:H	1.52	0.74
1:B:121:ASP:OD1	1:B:151:LYS:NZ	2.20	0.74
1:B:70:GLU:O	1:B:70:GLU:HG3	1.88	0.74
1:B:199:ILE:HD11	1:B:203:LEU:CD2	2.18	0.73
1:B:119:PHE:HD2	1:B:120:GLY:H	1.35	0.73
1:A:213:ASP:OD1	1:A:215:THR:HG23	1.88	0.73
1:B:199:ILE:HG12	1:B:203:LEU:CD2	2.17	0.72
1:A:251:VAL:CG2	1:A:252:GLU:N	2.52	0.72
1:B:221:LYS:O	1:B:225:ILE:HG23	1.90	0.71
1:B:197:ASN:OD1	1:B:197:ASN:N	2.23	0.71
1:A:45:LYS:CE	1:A:46:GLU:H	2.02	0.70
1:A:52:VAL:HG22	1:A:142:ILE:CG2	2.22	0.69
1:B:42:ASN:O	1:B:44:ASN:N	2.26	0.68
1:A:91:ARG:NH1	1:A:112:GLN:HE22	1.87	0.68
1:B:77:ILE:HG13	1:B:78:ASN:CG	2.13	0.68
1:B:194:ILE:HA	1:B:198:ASN:HD21	1.59	0.68
1:A:91:ARG:HH11	1:A:112:GLN:NE2	1.86	0.68
1:A:60:HIS:HB3	1:A:64:LYS:NZ	2.10	0.67
1:A:186:ILE:HD13	1:A:191:ILE:HB	1.76	0.67
1:A:113:PRO:HG3	1:A:142:ILE:HD11	1.77	0.67
1:B:42:ASN:C	1:B:44:ASN:H	1.97	0.66
1:B:23:TRP:O	1:B:27:GLU:HG3	1.95	0.65
1:A:186:ILE:O	1:A:187:ASP:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LYS:HG3	1:B:229:LYS:O	1.95	0.65
1:A:45:LYS:CE	1:A:46:GLU:N	2.59	0.64
1:B:250:GLU:O	1:B:252:GLU:HG2	1.98	0.64
1:B:77:ILE:HD12	1:B:78:ASN:H	1.61	0.64
1:B:233:PHE:CZ	1:B:251:VAL:HG12	2.33	0.64
1:A:54:GLY:HA3	2:A:300:IS3:S6	2.38	0.63
1:B:13:SER:O	1:B:22:LYS:HE2	1.99	0.63
1:B:174:LEU:HD11	1:B:176:LEU:HD21	1.81	0.62
1:B:193:ARG:HG2	1:B:194:ILE:N	2.14	0.62
1:A:229:LYS:O	1:A:259:SER:HA	2.01	0.61
1:B:199:ILE:CG1	1:B:203:LEU:CD2	2.78	0.61
1:A:158:SER:HB2	2:A:300:IS3:O3	2.00	0.61
1:B:227:LYS:O	1:B:228:ASN:CG	2.39	0.60
3:B:302:SO4:O1	4:B:286:HOH:O	2.15	0.60
1:A:164:PRO:HG3	1:A:224:MET:HG3	1.83	0.60
1:B:77:ILE:HD11	1:B:78:ASN:OD1	2.02	0.60
1:B:167:ALA:CB	1:B:175:ILE:HD11	2.30	0.59
1:A:17:VAL:O	1:A:20:SER:HB3	2.02	0.59
1:A:212:ILE:N	1:A:212:ILE:HD12	2.00	0.59
1:B:225:ILE:HD12	1:B:230:CYS:HB2	1.85	0.59
1:A:188:ASN:O	1:A:189:LYS:HG3	2.02	0.58
1:A:95:ASN:ND2	1:B:91:ARG:HH21	2.00	0.58
1:B:118:VAL:HG13	1:B:148:ILE:HG22	1.85	0.58
1:B:193:ARG:CG	1:B:194:ILE:N	2.66	0.58
1:B:194:ILE:O	1:B:194:ILE:HG22	2.02	0.58
1:B:14:ASP:OD1	1:B:14:ASP:C	2.42	0.58
1:B:196:LYS:HE2	1:B:197:ASN:OD1	2.05	0.56
1:B:252:GLU:OE1	1:B:252:GLU:HA	2.06	0.56
1:A:25:ASN:HD21	1:A:28:ARG:HH21	1.53	0.56
1:B:59:GLY:N	1:B:90:MET:HE1	2.20	0.56
1:A:25:ASN:ND2	1:A:28:ARG:HH21	2.04	0.56
1:A:142:ILE:HG13	1:A:143:HIS:N	2.21	0.56
1:A:109:VAL:HG11	1:B:83:PHE:CD2	2.41	0.55
1:A:199:ILE:HG23	1:A:200:TYR:H	1.69	0.55
1:B:227:LYS:O	1:B:228:ASN:CB	2.54	0.55
1:B:67:LEU:HD22	1:B:74:LYS:HB2	1.89	0.55
1:B:13:SER:OG	1:B:57:ALA:CB	2.55	0.54
1:A:91:ARG:HE	1:B:95:ASN:ND2	2.00	0.54
1:A:59:GLY:C	2:A:300:IS3:H4A	2.27	0.54
1:B:119:PHE:CG	1:B:155:ARG:HD3	2.41	0.54
1:B:53:HIS:NE2	1:B:143:HIS:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:HD12	1:A:172:ALA:HA	1.89	0.54
1:A:95:ASN:HD22	1:B:91:ARG:HH21	1.54	0.54
1:A:169:GLU:CG	4:A:294:HOH:O	2.55	0.53
1:B:228:ASN:O	1:B:229:LYS:HG2	2.07	0.53
1:A:9[B]:GLY:N	3:A:303:SO4:O3	2.42	0.53
1:A:186:ILE:O	1:A:187:ASP:CB	2.56	0.53
1:A:259:SER:O	1:A:260:GLU:HB2	2.08	0.53
1:B:54:GLY:CA	2:B:300:IS3:O	2.57	0.53
1:B:25:ASN:HD21	1:B:28:ARG:HH21	1.57	0.53
1:B:119:PHE:HE1	1:B:157:ILE:HG13	1.74	0.52
1:B:225:ILE:HD12	1:B:225:ILE:O	2.10	0.52
1:A:8[B]:GLY:O	1:A:11:ILE:HG12	2.08	0.52
1:B:60:HIS:O	1:B:61:PRO:C	2.41	0.52
1:B:42:ASN:C	1:B:44:ASN:N	2.63	0.52
1:B:228:ASN:O	1:B:229:LYS:CG	2.58	0.52
1:A:81:LYS:HD3	1:B:102:GLN:HE22	1.74	0.52
1:A:111:ILE:CG2	1:A:142:ILE:HD12	2.39	0.52
1:A:129:ALA:O	1:A:133:MET:HG3	2.10	0.52
1:A:199:ILE:CD1	1:A:226:ARG:HE	2.18	0.52
1:A:170:LEU:O	1:A:171:LYS:HB2	2.10	0.51
1:A:60:HIS:HB3	1:A:64:LYS:HZ3	1.74	0.51
1:A:8[A]:GLY:O	1:A:9[A]:GLY:C	2.46	0.51
1:A:175:ILE:O	1:A:232:GLY:HA2	2.10	0.51
1:B:195:ASP:HB3	1:B:197:ASN:OD1	2.10	0.51
1:A:111:ILE:HG22	1:A:142:ILE:HD12	1.92	0.51
1:B:68:LYS:O	1:B:75:ILE:N	2.43	0.51
1:A:102:GLN:OE1	1:B:81:LYS:HD3	2.11	0.51
1:B:199:ILE:HG12	1:B:199:ILE:O	2.09	0.51
1:B:5:LEU:HD13	1:B:7:LEU:HD21	1.93	0.51
1:A:159:GLY:O	1:A:163:VAL:HG23	2.11	0.50
1:B:70:GLU:HB3	1:B:75:ILE:HG12	1.91	0.50
1:B:150:ASP:OD1	1:B:151:LYS:N	2.44	0.50
1:A:60:HIS:HB2	1:A:61:PRO:HD3	1.93	0.50
1:A:81:LYS:HD3	1:B:102:GLN:NE2	2.27	0.50
1:A:6:LYS:CE	3:A:303:SO4:O4	2.58	0.50
1:A:1:MET:CE	1:A:3:THR:OG1	2.60	0.50
1:A:84:TRP:CD1	1:B:102:GLN:HG3	2.46	0.50
1:B:226:ARG:O	1:B:228:ASN:N	2.45	0.50
1:A:43:GLN:O	1:A:44:ASN:C	2.49	0.50
1:B:119:PHE:CE2	1:B:155:ARG:NE	2.80	0.50
1:A:55:GLY:N	2:A:300:IS3:H1A	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASN:HB2	1:A:228:ASN:HD21	1.78	0.49
1:A:28:ARG:HA	1:A:31:MET:CE	2.41	0.49
1:A:199:ILE:O	1:A:202:ILE:N	2.45	0.49
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.76	0.49
1:B:195:ASP:CB	1:B:197:ASN:OD1	2.60	0.49
1:A:28:ARG:O	1:A:32:GLU:HG3	2.12	0.49
1:B:167:ALA:CB	1:B:175:ILE:CD1	2.90	0.49
1:B:38:ASP:O	1:B:39:TYR:C	2.49	0.49
1:A:158:SER:HB2	2:A:300:IS3:P1	2.53	0.48
1:B:225:ILE:CD1	1:B:230:CYS:HB2	2.42	0.48
1:A:227:LYS:HG2	1:A:227:LYS:O	2.12	0.48
1:B:25:ASN:ND2	1:B:28:ARG:HH21	2.11	0.48
1:B:77:ILE:HG13	1:B:78:ASN:N	2.29	0.48
1:A:164:PRO:HB3	1:A:224:MET:CE	2.44	0.48
1:A:227:LYS:O	1:A:227:LYS:CG	2.61	0.48
1:A:2:LEU:HD22	1:A:3:THR:N	2.29	0.48
1:A:95:ASN:HD21	1:B:91:ARG:HE	1.62	0.48
1:A:251:VAL:CG2	1:A:252:GLU:H	2.25	0.48
1:B:136:ARG:HG3	1:B:136:ARG:NH1	2.29	0.48
1:B:127:THR:O	1:B:128:SER:C	2.51	0.47
1:A:28:ARG:HA	1:A:31:MET:HE3	1.96	0.47
1:B:32:GLU:HB3	1:B:244:TYR:HB2	1.95	0.47
1:A:203:LEU:HD13	1:A:223:GLU:OE2	2.15	0.47
1:B:239:LYS:O	1:B:240:ALA:C	2.52	0.47
1:B:179:THR:HB	3:B:301:SO4:O4	2.15	0.47
1:A:163:VAL:CB	1:A:164:PRO:CD	2.87	0.47
1:A:80:GLU:HB2	1:B:107:PRO:HB3	1.96	0.47
1:B:158:SER:HB2	2:B:300:IS3:P1	2.55	0.47
1:B:92:ARG:HG3	4:B:276:HOH:O	2.15	0.46
1:A:246:ALA:HA	1:A:251:VAL:HG12	1.97	0.46
1:B:77:ILE:CD1	1:B:78:ASN:OD1	2.64	0.46
1:A:186:ILE:HG22	1:A:187:ASP:OD2	2.16	0.46
1:A:169:GLU:HG3	4:A:294:HOH:O	2.13	0.46
1:A:1:MET:HE3	1:A:3:THR:OG1	2.16	0.46
1:B:13:SER:OG	1:B:57:ALA:HB2	2.15	0.46
1:B:195:ASP:HB2	1:B:197:ASN:H	1.81	0.46
1:B:77:ILE:CG1	1:B:78:ASN:N	2.79	0.46
1:B:136:ARG:N	1:B:136:ARG:HD3	2.31	0.45
1:A:2:LEU:HD13	1:A:172:ALA:CB	2.46	0.45
1:A:226:ARG:NH1	1:A:226:ARG:HG2	2.32	0.45
1:B:53:HIS:CE1	1:B:143:HIS:HB3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:O	1:A:39:TYR:C	2.55	0.45
1:A:226:ARG:HH11	1:A:226:ARG:HG2	1.81	0.44
1:A:136:ARG:O	1:A:137:ASN:CB	2.62	0.44
1:B:174:LEU:CD1	1:B:176:LEU:HD21	2.47	0.44
1:A:15:LYS:HB2	1:A:15:LYS:HE3	1.61	0.44
1:B:102:GLN:NE2	4:B:271:HOH:O	2.50	0.44
1:B:167:ALA:HB1	1:B:175:ILE:CD1	2.41	0.44
1:A:114:SER:HB3	1:A:146:ILE:O	2.17	0.44
1:B:3:THR:HG22	1:B:4:ILE:N	2.33	0.44
1:A:2:LEU:CD1	1:A:172:ALA:HA	2.48	0.44
1:B:9:GLY:O	1:B:13:SER:HB3	2.17	0.44
1:B:199:ILE:HG23	1:B:200:TYR:N	2.32	0.44
1:B:90:MET:CE	1:B:90:MET:N	2.81	0.44
1:B:136:ARG:O	1:B:137:ASN:HB2	2.16	0.43
1:A:109:VAL:CG1	1:B:83:PHE:CD2	3.01	0.43
1:B:227:LYS:HE2	1:B:227:LYS:HB3	1.46	0.43
1:B:119:PHE:CE1	1:B:157:ILE:HG13	2.52	0.43
1:B:54:GLY:HA3	2:B:300:IS3:P2	2.57	0.43
1:A:2:LEU:CD1	1:A:172:ALA:HB2	2.48	0.43
1:A:60:HIS:N	2:A:300:IS3:H4A	2.34	0.43
1:A:55:GLY:HA2	1:A:90:MET:CE	2.48	0.43
1:B:118:VAL:HB	1:B:124:ILE:HD12	2.00	0.43
1:A:227:LYS:HB2	1:A:227:LYS:NZ	2.32	0.43
1:B:240:ALA:O	1:B:241:ASN:CB	2.54	0.43
1:B:198:ASN:HD22	1:B:202:ILE:HD12	1.83	0.43
1:B:69:ILE:HA	1:B:69:ILE:HD13	1.88	0.43
1:B:86:ILE:HG21	1:B:86:ILE:HD13	1.86	0.43
1:B:223:GLU:O	1:B:226:ARG:N	2.52	0.42
1:B:149:ASP:O	1:B:153:GLY:N	2.46	0.42
1:B:160:ASP:O	1:B:164:PRO:CD	2.67	0.42
1:A:163:VAL:CB	1:A:164:PRO:HD3	2.41	0.42
1:B:186:ILE:N	1:B:189:LYS:O	2.45	0.42
1:A:126:ASP:OD1	1:A:128:SER:OG	2.27	0.42
1:A:164:PRO:HB3	1:A:224:MET:HE3	2.00	0.42
1:B:8:GLY:O	1:B:11:ILE:HG12	2.20	0.42
1:A:45:LYS:HE3	1:A:45:LYS:HA	2.02	0.41
1:A:47:ILE:O	1:A:47:ILE:HG23	2.20	0.41
1:A:2:LEU:CD1	1:A:172:ALA:CB	2.98	0.41
1:B:177:TYR:CD1	1:B:221:LYS:HE3	2.55	0.41
1:B:6:LYS:HE3	1:B:159:GLY:HA3	2.02	0.41
1:A:164:PRO:CG	1:A:224:MET:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:TYR:O	1:A:43:GLN:HG2	2.20	0.41
1:A:199:ILE:O	1:A:200:TYR:C	2.59	0.41
1:B:245:LYS:HE2	4:B:262:HOH:O	2.20	0.41
1:A:226:ARG:HD3	1:A:258:PHE:CE1	2.56	0.41
1:A:52:VAL:HA	1:A:142:ILE:O	2.21	0.41
1:B:189:LYS:HG3	1:B:190:PRO:HD2	2.03	0.41
1:A:227:LYS:HZ3	1:A:227:LYS:HB2	1.86	0.41
1:B:148:ILE:HA	1:B:148:ILE:HD13	1.79	0.41
1:B:180:ASP:N	1:B:180:ASP:OD1	2.48	0.41
1:A:225:ILE:HD13	1:A:232:GLY:HA3	2.02	0.41
1:B:220:TYR:O	1:B:224:MET:HB2	2.20	0.41
1:A:200:TYR:O	1:A:201:LYS:C	2.59	0.40
1:A:205:TYR:C	1:A:205:TYR:CD2	2.93	0.40
1:A:5:LEU:HD23	1:A:51:LEU:CD2	2.52	0.40
1:A:60:HIS:HB3	1:A:64:LYS:HZ2	1.86	0.40
1:B:146:ILE:O	1:B:146:ILE:HG23	2.21	0.40
1:B:199:ILE:O	1:B:203:LEU:HD22	2.22	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	261/266 (98%)	236 (90%)	23 (9%)	2 (1%)	22	23
1	B	244/266 (92%)	217 (89%)	21 (9%)	6 (2%)	6	4
All	All	505/532 (95%)	453 (90%)	44 (9%)	8 (2%)	11	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	GLN

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Mol	Chain	Res	Type
1	B	71	ASP
1	B	228	ASN
1	B	73	LYS
1	B	122	LYS
1	B	251	VAL
1	A	187	ASP
1	A	72	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	229/231 (99%)	217 (95%)	12 (5%)	27	33
1	B	219/231 (95%)	195 (89%)	24 (11%)	7	6
All	All	448/462 (97%)	412 (92%)	36 (8%)	14	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	15	LYS
1	A	45	LYS
1	A	123	LEU
1	A	125	PHE
1	A	137	ASN
1	A	155	ARG
1	A	185	LEU
1	A	212	ILE
1	A	215	THR
1	A	239	LYS
1	A	260	GLU
1	B	5	LEU
1	B	25	ASN
1	B	41	LYS
1	B	42	ASN

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Mol	Chain	Res	Type
1	B	45	LYS
1	B	47	ILE
1	B	64	LYS
1	B	73	LYS
1	B	74	LYS
1	B	92	ARG
1	B	95	ASN
1	B	119	PHE
1	B	125	PHE
1	B	142	ILE
1	B	148	ILE
1	B	191	ILE
1	B	192	LYS
1	B	196	LYS
1	B	197	ASN
1	B	199	ILE
1	B	201	LYS
1	B	221	LYS
1	B	224	MET
1	B	225	ILE

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	25	ASN
1	A	94	ASN
1	A	95	ASN
1	A	112	GLN
1	A	210	ASN
1	A	228	ASN
1	A	238	ASN
1	A	241	ASN
1	A	242	ASN
1	B	25	ASN
1	B	87	GLN
1	B	94	ASN
1	B	95	ASN
1	B	102	GLN
1	B	188	ASN
1	B	198	ASN
1	B	228	ASN
1	B	242	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
2	IS3	A	300	-	9,13,13	1.15	1 (11%)	11,19,19	1.47	1 (9%)
3	SO4	A	303	-	4,4,4	0.25	0	6,6,6	0.59	0
3	SO4	A	304	-	4,4,4	0.28	0	6,6,6	0.49	0
2	IS3	B	300	-	9,13,13	1.13	1 (11%)	11,19,19	1.58	2 (18%)
3	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.30	0
3	SO4	B	302	-	4,4,4	0.40	0	6,6,6	0.56	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	IS3	A	300	-	-	0/11/13/13	0/0/0/0
3	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	IS3	B	300	-	-	0/11/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	301	-	-	0/0/0/0	0/0/0/0
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	IS3	C5-C3	-3.19	1.33	1.51
2	B	300	IS3	C5-C3	-3.09	1.34	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	IS3	C5-C3-C4	2.11	120.48	110.50
2	B	300	IS3	O5-P2-O4	2.66	115.52	109.87
2	A	300	IS3	O5-P2-O4	3.23	116.72	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	IS3	6	0
3	A	303	SO4	5	0
2	B	300	IS3	5	0
3	B	301	SO4	1	0
3	B	302	SO4	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

### 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	260/266 (97%)	0.28	12 (4%) 33 44	25, 45, 66, 76	0
1	B	248/266 (93%)	0.84	37 (14%) 3 4	28, 54, 82, 93	0
All	All	508/532 (95%)	0.55	49 (9%) 9 14	25, 49, 76, 93	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	ASP	6.4
1	A	212	ILE	5.1
1	B	121	ASP	4.8
1	B	226	ARG	4.4
1	B	251	VAL	4.4
1	B	258	PHE	4.4
1	A	260	GLU	4.3
1	B	122	LYS	4.3
1	B	69	ILE	4.3
1	B	73	LYS	4.2
1	A	186	ILE	3.8
1	B	72	GLY	3.8
1	B	120	GLY	3.6
1	B	68	LYS	3.4
1	B	196	LYS	3.2
1	A	187	ASP	3.2
1	B	74	LYS	3.1
1	A	9[A]	GLY	3.0
1	B	219	LYS	3.0
1	B	70	GLU	2.9
1	B	198	ASN	2.9
1	A	98	ILE	2.8
1	B	89	ALA	2.7
1	B	143	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	46	GLU	2.7
1	B	195	ASP	2.7
1	B	194	ILE	2.6
1	B	220	TYR	2.6
1	A	188	ASN	2.6
1	B	200	TYR	2.6
1	B	90	MET	2.5
1	B	231	ARG	2.5
1	B	75	ILE	2.4
1	B	98	ILE	2.4
1	A	211	SER	2.3
1	B	192	LYS	2.3
1	B	202	ILE	2.3
1	A	189	LYS	2.2
1	B	233	PHE	2.2
1	B	96	ILE	2.2
1	B	141	VAL	2.2
1	B	193	ARG	2.2
1	A	1	MET	2.1
1	B	229	LYS	2.1
1	B	44	ASN	2.1
1	B	222	ILE	2.1
1	B	227	LYS	2.1
1	A	100	THR	2.1
1	B	94	ASN	2.1

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	301	5/5	0.79	0.24	3.45	126,126,126,127	0
3	SO4	B	302	5/5	0.91	0.20	2.93	132,133,133,134	0
2	IS3	B	300	14/14	0.93	0.15	-0.20	58,71,77,78	0
2	IS3	A	300	14/14	0.92	0.14	-0.39	60,63,68,71	0
3	SO4	A	304	5/5	0.98	0.14	-0.43	46,48,53,54	0
3	SO4	A	303	5/5	0.95	0.10	-1.05	76,77,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.