



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 11:20 PM EDT

PDB ID : 5J0A  
Title : Crystal structure of PDZ-binding kinase  
Authors : Zou, Q.W.; Zhou, H.; Yang, X.  
Deposited on : 2016-03-28  
Resolution : 2.74 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

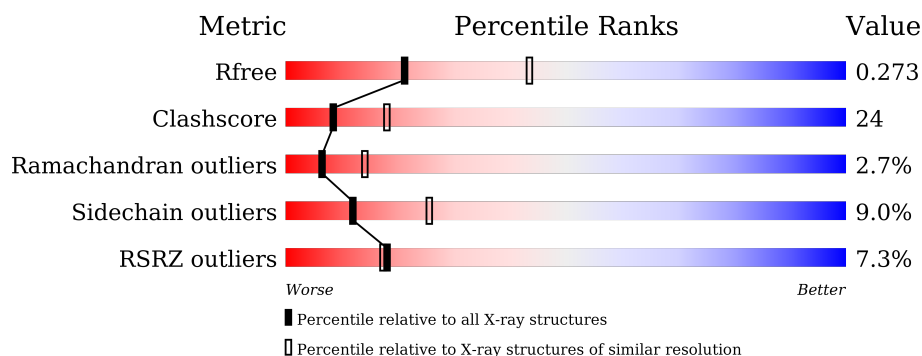
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	300	<div> <div>8%</div> <div>56%</div> <div>38%</div> <div>5%</div> </div>
2	B	304	<div> <div>7%</div> <div>52%</div> <div>41%</div> <div>6%</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
3	SO4	A	401	-	-	-	X
3	SO4	A	403	-	-	-	X
3	SO4	B	401	-	-	X	-
3	SO4	B	402	-	-	-	X
3	SO4	B	404	-	-	-	X
4	HC4	A	406	-	-	-	X
4	HC4	A	408	-	-	-	X
4	HC4	B	406	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4975 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 Lymphokine-activated killer T-cell-originated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2355	1490	387	464	14	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q96KB5
A	198	GLU	THR	engineered mutation	UNP Q96KB5
A	321	ALA	-	expression tag	UNP Q96KB5

- Molecule 2 is a protein called Lymphokine-activated killer T-cell-originated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	303	2380	1506	391	468	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

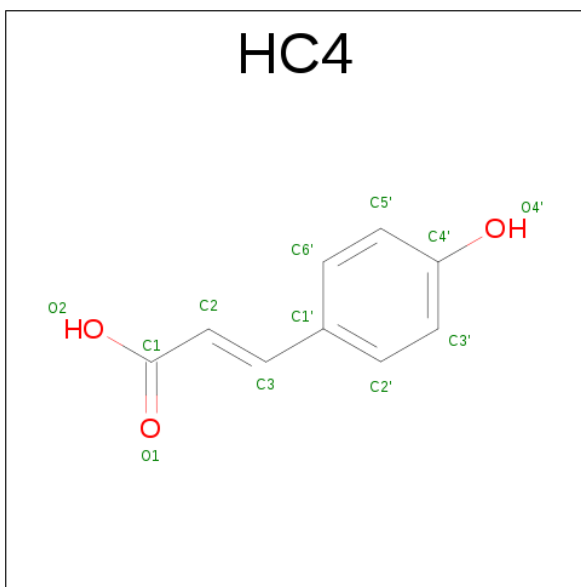
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLY	-	expression tag	UNP Q96KB5
B	198	GLU	THR	engineered mutation	UNP Q96KB5
B	320	ALA	-	expression tag	UNP Q96KB5
B	321	ALA	-	expression tag	UNP Q96KB5

- 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		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
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 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	A	1	Total	C	O	0	0
			12	9	3		
4	A	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

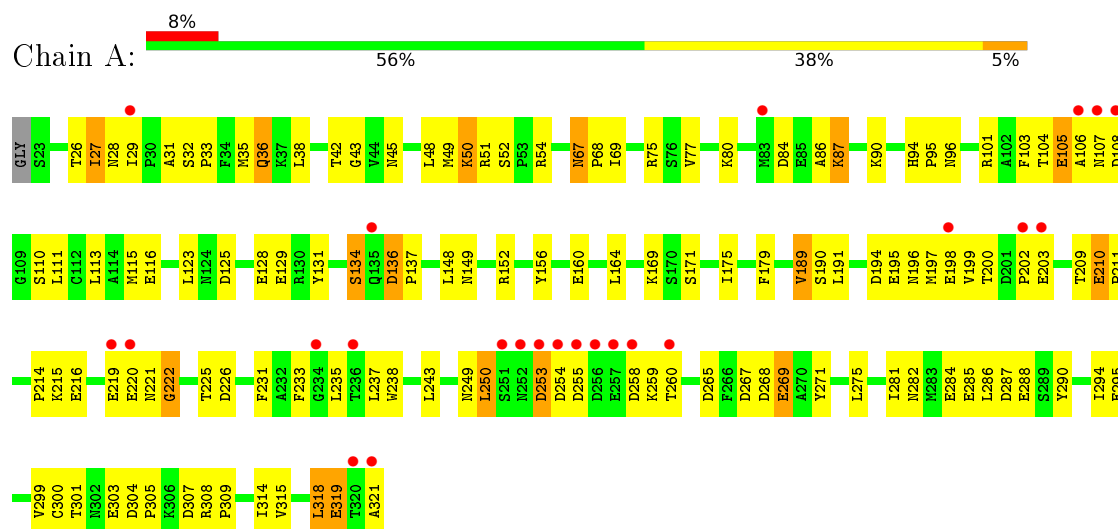
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	81	Total	O	0	0
			81	81		

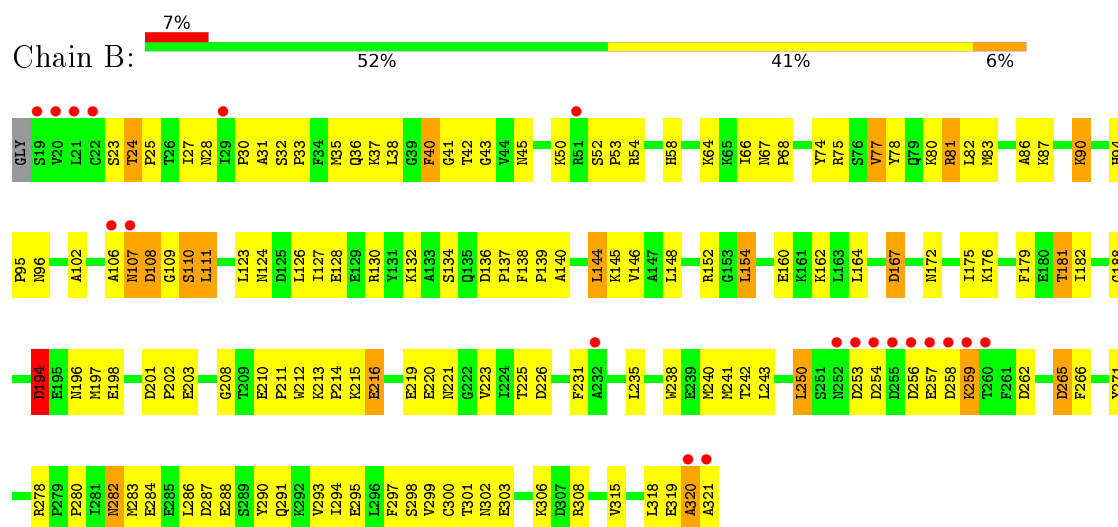
### 3 Residue-property plots

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

- Molecule 1: Lymphokine-activated killer T-cell-originated protein kinase



- Molecule 2: Lymphokine-activated killer T-cell-originated protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.56Å 97.91Å 162.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.76 – 2.74 32.76 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.6 (32.76-2.74) 95.7 (32.76-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.96 (at 2.72Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.222 , 0.271 0.226 , 0.273	Depositor DCC
$R_{free}$ test set	1580 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: SO4, HC4

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	0.35	0/2407	0.58	0/3262
2	B	0.39	0/2432	0.61	0/3296
All	All	0.37	0/4839	0.59	0/6558

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	2355	0	2303	112	0
2	B	2380	0	2331	134	0
3	A	25	0	0	2	0
3	B	25	0	0	3	0
4	A	36	0	18	3	0
4	B	12	0	6	0	0
5	A	61	0	0	2	0
5	B	81	0	0	4	0
All	All	4975	0	4658	228	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 24.

All (228) 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)
2:B:42:THR:HG22	2:B:43:GLY:H	1.21	1.02
2:B:198:GLU:HG2	2:B:225:THR:HG22	1.51	0.90
1:A:105:GLU:H	1:A:105:GLU:CD	1.78	0.88
1:A:94:HIS:HD2	1:A:96:ASN:H	1.19	0.87
2:B:167:ASP:HB3	2:B:208:GLY:HA2	1.59	0.84
2:B:167:ASP:CB	2:B:208:GLY:HA2	2.09	0.83
1:A:210:GLU:HB3	1:A:211:PRO:HD3	1.60	0.82
1:A:94:HIS:CD2	1:A:96:ASN:H	1.96	0.82
1:A:69:ILE:HD11	1:A:75:ARG:HG3	1.64	0.79
2:B:94:HIS:HD2	2:B:96:ASN:H	1.31	0.78
2:B:176:LYS:HB3	2:B:181:THR:HB	1.65	0.78
2:B:194:ASP:HB3	2:B:196:ASN:H	1.49	0.78
2:B:31:ALA:HA	2:B:42:THR:O	1.85	0.76
1:A:42:THR:HG22	1:A:43:GLY:O	1.85	0.76
1:A:250:LEU:HD12	1:A:250:LEU:H	1.50	0.76
2:B:194:ASP:HB2	2:B:198:GLU:H	1.50	0.76
2:B:94:HIS:CD2	2:B:96:ASN:H	2.04	0.76
1:A:267:ASP:OD1	1:A:269:GLU:HB2	1.85	0.75
1:A:52:SER:HB2	1:A:54:ARG:NH1	2.04	0.72
2:B:220:GLU:CD	2:B:220:GLU:H	1.91	0.72
1:A:50:LYS:H	1:A:50:LYS:HZ2	1.35	0.70
1:A:321:ALA:HB1	2:B:37:LYS:NZ	2.07	0.69
1:A:284:GLU:HG3	2:B:50:LYS:HA	1.75	0.69
2:B:181:THR:HG22	5:B:507:HOH:O	1.92	0.69
2:B:286:LEU:HD22	2:B:290:TYR:CD2	2.29	0.68
2:B:42:THR:HG22	2:B:43:GLY:N	2.01	0.68
2:B:75:ARG:HD2	3:B:403:SO4:O2	1.94	0.67
2:B:36:GLN:HA	2:B:41:GLY:N	2.08	0.67
2:B:215:LYS:NZ	2:B:303:GLU:HB3	2.09	0.67
1:A:87:LYS:HE3	1:A:87:LYS:HA	1.77	0.66
2:B:23:SER:O	2:B:24:THR:HG23	1.96	0.66
2:B:130:ARG:NH2	2:B:139:PRO:HD3	2.11	0.66
1:A:219:GLU:HB2	1:A:222:GLY:H	1.61	0.65
1:A:156:TYR:O	1:A:160:GLU:HB2	1.97	0.65
2:B:210:GLU:HA	2:B:213:LYS:HG3	1.78	0.65
1:A:32:SER:HB2	1:A:33:PRO:HD2	1.79	0.64
2:B:77:VAL:HG22	2:B:78:TYR:CD2	2.33	0.63
1:A:94:HIS:HD2	1:A:96:ASN:N	1.95	0.62
2:B:67:ASN:N	2:B:68:PRO:HD3	2.14	0.62
2:B:282:ASN:N	2:B:282:ASN:HD22	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:LEU:HD12	2:B:250:LEU:H	1.65	0.62
1:A:131:TYR:CE2	2:B:54:ARG:HB3	2.35	0.61
2:B:188:GLY:HA3	3:B:401:SO4:O4	2.00	0.61
2:B:176:LYS:CB	2:B:181:THR:HB	2.31	0.61
1:A:281:ILE:HD11	1:A:286:LEU:HD11	1.82	0.61
1:A:314:ILE:O	1:A:318:LEU:HB2	2.01	0.60
1:A:131:TYR:CD2	2:B:54:ARG:HB3	2.36	0.60
1:A:27:ILE:HG21	1:A:48:LEU:HD21	1.83	0.60
2:B:81:ARG:NH2	3:B:401:SO4:O1	2.33	0.60
1:A:290:TYR:O	1:A:294:ILE:HG13	2.02	0.60
1:A:197:MET:HG3	1:A:226:ASP:HB3	1.84	0.59
2:B:250:LEU:HA	2:B:265:ASP:O	2.02	0.59
1:A:214:PRO:HA	1:A:231:PHE:CD2	2.38	0.59
1:A:38:LEU:HD13	2:B:299:VAL:HG21	1.85	0.59
1:A:86:ALA:O	1:A:90:LYS:HG3	2.02	0.59
2:B:290:TYR:O	2:B:294:ILE:HG13	2.03	0.58
2:B:167:ASP:HB2	2:B:208:GLY:HA2	1.82	0.58
2:B:256:ASP:O	2:B:257:GLU:HB3	2.02	0.58
2:B:36:GLN:HA	2:B:41:GLY:H	1.68	0.58
2:B:25:PRO:HG2	2:B:50:LYS:NZ	2.18	0.58
2:B:278:ARG:NH1	2:B:298:SER:O	2.37	0.57
2:B:201:ASP:OD1	2:B:202:PRO:HD2	2.03	0.57
1:A:299:VAL:HG21	2:B:38:LEU:HD13	1.88	0.56
2:B:300:CYS:O	2:B:308:ARG:HD3	2.06	0.56
1:A:105:GLU:N	1:A:105:GLU:CD	2.54	0.56
2:B:278:ARG:HD3	2:B:301:THR:OG1	2.05	0.56
1:A:214:PRO:HA	1:A:231:PHE:CE2	2.42	0.55
1:A:50:LYS:N	1:A:50:LYS:HZ2	2.05	0.55
2:B:106:ALA:HB2	2:B:111:LEU:HG	1.89	0.55
2:B:215:LYS:HZ2	2:B:303:GLU:HB3	1.69	0.54
1:A:194:ASP:HB3	1:A:198:GLU:O	2.07	0.54
2:B:124:ASN:O	2:B:127:ILE:HG13	2.08	0.54
1:A:28:ASN:HA	1:A:45:ASN:HD22	1.72	0.54
1:A:169:LYS:HE3	1:A:171:SER:HB2	1.91	0.53
1:A:50:LYS:H	1:A:50:LYS:CD	2.21	0.52
1:A:67:ASN:N	1:A:68:PRO:HD3	2.24	0.52
2:B:145:LYS:HE2	2:B:179:PHE:O	2.09	0.52
1:A:194:ASP:CG	1:A:195:GLU:N	2.62	0.52
1:A:196:ASN:O	1:A:198:GLU:HG3	2.09	0.52
1:A:203:GLU:HA	1:A:203:GLU:OE2	2.09	0.52
2:B:215:LYS:O	2:B:219:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ALA:O	2:B:90:LYS:HB2	2.10	0.52
1:A:219:GLU:C	1:A:221:ASN:H	2.13	0.52
2:B:127:ILE:C	2:B:127:ILE:HD12	2.30	0.52
1:A:243:LEU:O	2:B:58:HIS:HE1	1.92	0.51
2:B:146:VAL:HA	2:B:182:ILE:HD13	1.92	0.51
1:A:164:LEU:HD13	1:A:226:ASP:HA	1.93	0.51
2:B:130:ARG:HH22	2:B:139:PRO:HD3	1.73	0.51
2:B:241:MET:HE3	2:B:293:VAL:HG12	1.92	0.51
2:B:259:LYS:HB2	5:B:542:HOH:O	2.11	0.51
1:A:321:ALA:HB1	2:B:37:LYS:CE	2.41	0.51
1:A:94:HIS:HD1	1:A:156:TYR:HB2	1.76	0.50
1:A:198:GLU:O	1:A:200:THR:HG23	2.10	0.50
1:A:107:ASN:OD1	1:A:108:ASP:N	2.45	0.50
2:B:256:ASP:O	2:B:257:GLU:CB	2.60	0.49
1:A:282:ASN:HD22	1:A:285:GLU:HB2	1.78	0.49
2:B:291:GLN:O	2:B:295:GLU:HG3	2.13	0.49
1:A:189:VAL:N	3:A:402:SO4:O3	2.44	0.49
2:B:167:ASP:HB2	5:B:537:HOH:O	2.13	0.49
1:A:300:CYS:O	1:A:308:ARG:HD2	2.12	0.49
1:A:50:LYS:HG2	1:A:51:ARG:H	1.76	0.49
2:B:80:LYS:HE3	2:B:110:SER:OG	2.13	0.49
2:B:318:LEU:C	2:B:320:ALA:H	2.15	0.49
2:B:278:ARG:HH12	2:B:302:ASN:ND2	2.11	0.48
1:A:101:ARG:HB3	1:A:116:GLU:OE1	2.13	0.48
2:B:259:LYS:HB3	2:B:259:LYS:NZ	2.28	0.48
2:B:75:ARG:HD3	2:B:75:ARG:HA	1.62	0.48
2:B:140:ALA:HB2	2:B:290:TYR:CD1	2.48	0.48
2:B:214:PRO:HB2	2:B:216:GLU:OE2	2.13	0.48
1:A:27:ILE:HG22	1:A:48:LEU:HG	1.96	0.47
1:A:50:LYS:H	1:A:50:LYS:HD3	1.79	0.47
1:A:49:MET:HE3	2:B:280:PRO:HG2	1.96	0.47
2:B:28:ASN:O	2:B:30:PRO:HD3	2.14	0.47
2:B:42:THR:CG2	2:B:43:GLY:H	2.04	0.47
1:A:115:MET:CE	2:B:74:TYR:HA	2.45	0.47
2:B:194:ASP:HB3	2:B:196:ASN:N	2.25	0.47
1:A:103:PHE:O	1:A:104:THR:HG23	2.14	0.47
2:B:94:HIS:CD2	2:B:95:PRO:HD2	2.50	0.47
1:A:225:THR:OG1	1:A:226:ASP:N	2.47	0.46
1:A:210:GLU:HB3	1:A:211:PRO:CD	2.39	0.46
1:A:258:ASP:OD2	1:A:260:THR:HB	2.15	0.46
2:B:148:LEU:HD21	2:B:152:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:O	1:A:219:GLU:HG2	2.16	0.46
2:B:137:PRO:O	2:B:138:PHE:C	2.52	0.46
2:B:32:SER:OG	2:B:33:PRO:HD2	2.16	0.46
2:B:287:ASP:OD1	2:B:288:GLU:N	2.49	0.46
1:A:104:THR:O	1:A:111:LEU:HD11	2.15	0.46
2:B:194:ASP:HB2	2:B:198:GLU:O	2.16	0.46
1:A:315:VAL:O	1:A:319:GLU:N	2.45	0.45
1:A:28:ASN:HB2	1:A:45:ASN:ND2	2.31	0.45
2:B:123:LEU:O	2:B:127:ILE:HG23	2.16	0.45
1:A:131:TYR:CD1	1:A:131:TYR:C	2.90	0.45
1:A:307:ASP:OD1	2:B:40:PHE:HE1	1.99	0.45
1:A:194:ASP:CG	1:A:195:GLU:H	2.19	0.45
1:A:80:LYS:HE2	1:A:110:SER:HB2	1.97	0.45
2:B:266:PHE:HZ	2:B:271:TYR:CG	2.34	0.45
1:A:152:ARG:HG3	3:A:405:SO4:S	2.57	0.45
2:B:315:VAL:O	2:B:319:GLU:HG3	2.16	0.45
1:A:321:ALA:HB1	2:B:37:LYS:HZ2	1.82	0.45
1:A:94:HIS:CD2	1:A:95:PRO:N	2.85	0.45
2:B:262:ASP:N	2:B:265:ASP:OD2	2.40	0.45
1:A:231:PHE:CD1	1:A:301:THR:HA	2.52	0.45
1:A:281:ILE:HD12	1:A:282:ASN:H	1.82	0.45
1:A:35:MET:HB2	2:B:295:GLU:OE1	2.16	0.45
4:A:408:HC4:H3'	5:A:505:HOH:O	2.16	0.44
2:B:258:ASP:O	2:B:259:LYS:C	2.55	0.44
2:B:137:PRO:HG3	2:B:241:MET:O	2.17	0.44
2:B:128:GLU:O	2:B:132:LYS:HG2	2.16	0.44
1:A:87:LYS:NZ	1:A:90:LYS:HE2	2.32	0.44
2:B:215:LYS:HZ1	2:B:303:GLU:HB3	1.80	0.44
2:B:28:ASN:ND2	2:B:45:ASN:OD1	2.51	0.44
1:A:304:ASP:HA	1:A:305:PRO:HD3	1.86	0.44
2:B:221:ASN:O	2:B:221:ASN:OD1	2.36	0.44
2:B:175:ILE:HD12	2:B:182:ILE:HG12	2.00	0.43
2:B:164:LEU:HD13	2:B:226:ASP:HA	2.00	0.43
2:B:90:LYS:HD2	2:B:102:ALA:HB2	2.00	0.43
1:A:235:LEU:O	1:A:238:TRP:HB3	2.18	0.43
2:B:108:ASP:CG	2:B:109:GLY:H	2.22	0.43
2:B:278:ARG:HH12	2:B:302:ASN:HD22	1.66	0.43
1:A:190:SER:O	1:A:191:LEU:HD23	2.18	0.43
2:B:212:TRP:HA	2:B:235:LEU:HD23	2.01	0.43
2:B:238:TRP:HB2	2:B:297:PHE:CE1	2.54	0.43
1:A:49:MET:HB2	2:B:280:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ASN:N	2:B:282:ASN:ND2	2.64	0.43
2:B:52:SER:HA	2:B:53:PRO:HD3	1.87	0.43
1:A:125:ASP:O	1:A:129:GLU:HB2	2.18	0.43
1:A:216:GLU:HA	1:A:219:GLU:CG	2.49	0.43
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.84	0.43
1:A:215:LYS:HD3	1:A:303:GLU:OE1	2.18	0.43
2:B:127:ILE:HG22	2:B:138:PHE:HE2	1.84	0.43
1:A:38:LEU:CD1	2:B:299:VAL:HG21	2.48	0.43
4:A:408:HC4:H2	2:B:66:ILE:HA	2.01	0.43
1:A:36:GLN:HG3	5:A:527:HOH:O	2.18	0.43
2:B:282:ASN:HD22	2:B:282:ASN:H	1.62	0.43
1:A:308:ARG:HA	1:A:309:PRO:HD3	1.94	0.42
1:A:94:HIS:ND1	1:A:156:TYR:HB2	2.34	0.42
2:B:64:LYS:HE3	2:B:64:LYS:HB2	1.87	0.42
1:A:216:GLU:OE1	1:A:308:ARG:NH2	2.52	0.42
2:B:198:GLU:CG	2:B:225:THR:HG22	2.37	0.42
1:A:175:ILE:HG12	1:A:179:PHE:CE1	2.54	0.42
2:B:201:ASP:OD1	2:B:202:PRO:CD	2.66	0.42
1:A:209:THR:HG22	1:A:211:PRO:HD2	2.02	0.42
1:A:216:GLU:HA	1:A:219:GLU:HG2	2.02	0.42
2:B:126:LEU:C	2:B:128:GLU:H	2.23	0.42
2:B:27:ILE:HG12	2:B:28:ASN:N	2.35	0.42
2:B:126:LEU:C	2:B:128:GLU:N	2.73	0.42
2:B:36:GLN:OE1	2:B:41:GLY:HA3	2.19	0.42
2:B:77:VAL:HG22	2:B:78:TYR:CE2	2.54	0.42
1:A:94:HIS:HD1	1:A:156:TYR:CB	2.32	0.42
2:B:162:LYS:CD	2:B:197:MET:HE1	2.50	0.42
2:B:238:TRP:CE2	2:B:242:THR:HG21	2.55	0.42
1:A:282:ASN:ND2	1:A:285:GLU:OE1	2.50	0.41
1:A:50:LYS:H	1:A:50:LYS:NZ	2.11	0.41
2:B:181:THR:CG2	5:B:507:HOH:O	2.60	0.41
2:B:83:MET:HE2	2:B:87:LYS:HE3	2.02	0.41
1:A:219:GLU:O	1:A:220:GLU:HB3	2.20	0.41
1:A:80:LYS:HE2	1:A:110:SER:CB	2.51	0.41
1:A:96:ASN:OD1	1:A:149:ASN:HB3	2.21	0.41
1:A:282:ASN:ND2	1:A:285:GLU:HB2	2.34	0.41
2:B:320:ALA:O	2:B:321:ALA:HB3	2.20	0.41
1:A:295:GLU:OE1	2:B:35:MET:HG3	2.21	0.41
1:A:233:PHE:CE1	1:A:237:LEU:HD11	2.55	0.41
1:A:48:LEU:CD2	2:B:283:MET:HB2	2.50	0.41
2:B:144:LEU:HD22	2:B:293:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LEU:HA	2:B:154:LEU:HD12	1.92	0.41
2:B:242:THR:O	2:B:243:LEU:HB2	2.21	0.41
2:B:250:LEU:HD12	2:B:250:LEU:N	2.33	0.41
1:A:284:GLU:H	1:A:284:GLU:HG2	1.66	0.41
4:A:408:HC4:H2	4:A:408:HC4:H6'	1.81	0.41
2:B:123:LEU:HD11	2:B:240:MET:HE3	2.02	0.41
1:A:77:VAL:HG22	2:B:77:VAL:HB	2.02	0.41
1:A:287:ASP:OD1	1:A:288:GLU:N	2.54	0.41
1:A:36:GLN:HE21	1:A:36:GLN:HA	1.84	0.41
1:A:94:HIS:CD2	1:A:95:PRO:HD2	2.56	0.41
2:B:94:HIS:CG	2:B:95:PRO:HD2	2.56	0.41
1:A:94:HIS:CD2	1:A:94:HIS:C	2.94	0.41
1:A:134:SER:HB2	1:A:136:ASP:H	1.86	0.40
1:A:29:ILE:O	1:A:43:GLY:HA2	2.21	0.40
2:B:134:SER:C	2:B:136:ASP:H	2.25	0.40
1:A:219:GLU:C	1:A:221:ASN:N	2.74	0.40
1:A:253:ASP:O	1:A:254:ASP:CB	2.69	0.40
2:B:210:GLU:CB	2:B:211:PRO:HD3	2.52	0.40
2:B:282:ASN:H	2:B:282:ASN:ND2	2.18	0.40
1:A:137:PRO:HD3	2:B:54:ARG:HH22	1.86	0.40
2:B:83:MET:O	2:B:87:LYS:HG3	2.21	0.40
2:B:231:PHE:CD1	2:B:301:THR:HA	2.57	0.40
1:A:131:TYR:HE2	2:B:54:ARG:HB3	1.85	0.40
2:B:203:GLU:HA	2:B:203:GLU:OE2	2.22	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	297/300 (99%)	254 (86%)	32 (11%)	11 (4%)	<b>4</b> <b>8</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	301/304 (99%)	265 (88%)	31 (10%)	5 (2%)	11	27
All	All	598/604 (99%)	519 (87%)	63 (10%)	16 (3%)	6	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
2	B	107	ASN
1	A	269	GLU
1	A	275	LEU
2	B	259	LYS
1	A	31	ALA
2	B	108	ASP
2	B	320	ALA
1	A	210	GLU
1	A	253	ASP
1	A	271	TYR
1	A	106	ALA
2	B	194	ASP
1	A	199	VAL
1	A	202	PRO
1	A	222	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	261/261 (100%)	239 (92%)	22 (8%)	14	29
2	B	264/264 (100%)	239 (90%)	25 (10%)	11	23
All	All	525/525 (100%)	478 (91%)	47 (9%)	12	25

All (47) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	26	THR
1	A	27	ILE
1	A	36	GLN
1	A	50	LYS
1	A	67	ASN
1	A	84	ASP
1	A	87	LYS
1	A	105	GLU
1	A	113	LEU
1	A	123	LEU
1	A	128	GLU
1	A	134	SER
1	A	136	ASP
1	A	148	LEU
1	A	189	VAL
1	A	249	ASN
1	A	250	LEU
1	A	255	ASP
1	A	259	LYS
1	A	265	ASP
1	A	268	ASP
1	A	318	LEU
2	B	24	THR
2	B	40	PHE
2	B	77	VAL
2	B	81	ARG
2	B	82	LEU
2	B	90	LYS
2	B	107	ASN
2	B	110	SER
2	B	111	LEU
2	B	144	LEU
2	B	154	LEU
2	B	160	GLU
2	B	167	ASP
2	B	172	ASN
2	B	181	THR
2	B	194	ASP
2	B	216	GLU
2	B	223	VAL
2	B	250	LEU
2	B	253	ASP
2	B	254	ASP

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Mol	Chain	Res	Type
2	B	265	ASP
2	B	282	ASN
2	B	284	GLU
2	B	306	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	36	GLN
1	A	45	ASN
1	A	67	ASN
1	A	79	GLN
1	A	302	ASN
2	B	79	GLN
2	B	94	HIS
2	B	107	ASN
2	B	172	ASN
2	B	282	ASN
2	B	302	ASN

### 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](#)

14 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	A	401	-	4,4,4	0.90	0	6,6,6	0.06	0
3	SO4	A	402	-	4,4,4	0.89	0	6,6,6	1.71	2 (33%)
3	SO4	A	403	-	4,4,4	0.89	0	6,6,6	0.05	0
3	SO4	A	404	-	4,4,4	0.88	0	6,6,6	0.07	0
3	SO4	A	405	-	4,4,4	0.89	0	6,6,6	0.06	0
4	HC4	A	406	-	9,12,12	1.05	1 (11%)	11,15,15	0.75	0
4	HC4	A	407	-	9,12,12	1.05	1 (11%)	11,15,15	0.73	0
4	HC4	A	408	-	9,12,12	1.10	1 (11%)	11,15,15	0.70	0
3	SO4	B	401	-	4,4,4	0.89	0	6,6,6	0.07	0
3	SO4	B	402	-	4,4,4	0.89	0	6,6,6	0.07	0
3	SO4	B	403	-	4,4,4	0.89	0	6,6,6	0.06	0
3	SO4	B	404	-	4,4,4	0.89	0	6,6,6	0.05	0
3	SO4	B	405	-	4,4,4	0.89	0	6,6,6	0.06	0
4	HC4	B	406	-	9,12,12	1.05	1 (11%)	11,15,15	0.69	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
3	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	SO4	A	405	-	-	0/0/0/0	0/0/0/0
4	HC4	A	406	-	-	0/3/5/5	0/1/1/1
4	HC4	A	407	-	-	0/3/5/5	0/1/1/1
4	HC4	A	408	-	-	0/3/5/5	0/1/1/1
3	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	SO4	B	403	-	-	0/0/0/0	0/0/0/0
3	SO4	B	404	-	-	0/0/0/0	0/0/0/0
3	SO4	B	405	-	-	0/0/0/0	0/0/0/0
4	HC4	B	406	-	-	0/3/5/5	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	HC4	C1'-C3	-2.77	1.39	1.47
4	B	406	HC4	C1'-C3	-2.65	1.39	1.47
4	A	407	HC4	C1'-C3	-2.65	1.39	1.47
4	A	406	HC4	C1'-C3	-2.62	1.39	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	SO4	O2-S-O1	-2.64	100.78	109.59
3	A	402	SO4	O4-S-O3	2.54	119.32	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	1	0
3	A	405	SO4	1	0
4	A	408	HC4	3	0
3	B	401	SO4	2	0
3	B	403	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	299/300 (99%)	0.36	24 (8%) 15 14	38, 74, 107, 132	0
2	B	303/304 (99%)	0.29	20 (6%) 22 21	36, 60, 107, 129	0
All	All	602/604 (99%)	0.33	44 (7%) 18 17	36, 67, 107, 132	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ASP	5.8
2	B	19	SER	5.3
1	A	256	ASP	5.2
2	B	257	GLU	4.8
2	B	254	ASP	4.8
2	B	21	LEU	4.5
2	B	22	CYS	4.2
1	A	320	THR	3.9
1	A	321	ALA	3.9
2	B	51	ARG	3.8
2	B	260	THR	3.8
2	B	252	ASN	3.6
1	A	254	ASP	3.5
2	B	256	ASP	3.3
1	A	135	GLN	3.3
2	B	320	ALA	3.2
1	A	234	GLY	3.2
2	B	258	ASP	3.1
2	B	255	ASP	3.1
2	B	253	ASP	3.0
2	B	259	LYS	3.0
2	B	106	ALA	3.0
2	B	20	VAL	3.0
1	A	83	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	2.9
2	B	232	ALA	2.8
2	B	107	ASN	2.8
2	B	321	ALA	2.7
1	A	252	ASN	2.6
1	A	202	PRO	2.5
1	A	198	GLU	2.5
1	A	107	ASN	2.5
1	A	251	SER	2.5
1	A	219	GLU	2.4
1	A	257	GLU	2.4
2	B	29	ILE	2.3
1	A	203	GLU	2.3
1	A	258	ASP	2.2
1	A	108	ASP	2.2
1	A	253	ASP	2.2
1	A	236	THR	2.1
1	A	220	GLU	2.1
1	A	29	ILE	2.0
1	A	260	THR	2.0

## 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
3	SO4	B	402	5/5	0.86	0.35	13.11	140,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	401	5/5	0.83	0.30	10.58	133,133,134,134	0
4	HC4	A	408	12/12	0.73	0.38	5.65	60,82,87,87	0
3	SO4	A	403	5/5	0.81	0.37	5.11	134,135,135,136	0
3	SO4	B	404	5/5	0.77	0.28	3.87	138,139,139,140	0
4	HC4	B	406	12/12	0.86	0.28	2.72	87,91,96,97	0
4	HC4	A	406	12/12	0.83	0.26	2.32	40,59,62,62	0
3	SO4	B	405	5/5	0.92	0.21	0.64	129,129,129,130	0
4	HC4	A	407	12/12	0.98	0.16	0.46	36,39,45,46	0
3	SO4	B	401	5/5	0.98	0.10	-2.01	71,72,73,75	0
3	SO4	A	405	5/5	0.78	0.46	-	148,148,149,149	0
3	SO4	B	403	5/5	0.91	0.29	-	112,112,113,113	0
3	SO4	A	402	5/5	0.97	0.10	-	80,80,81,82	0
3	SO4	A	404	5/5	0.93	0.23	-	138,138,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.