



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:34 am BST

PDB ID : 2ZW6
Title : Crystal structure of bleomycin N-acetyltransferase from bleomycin-producing *Streptomyces verticillus* ATCC15003
Authors : Oda, K.; Matoba, Y.; Sugiyama, M.
Deposited on : 2008-12-01
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

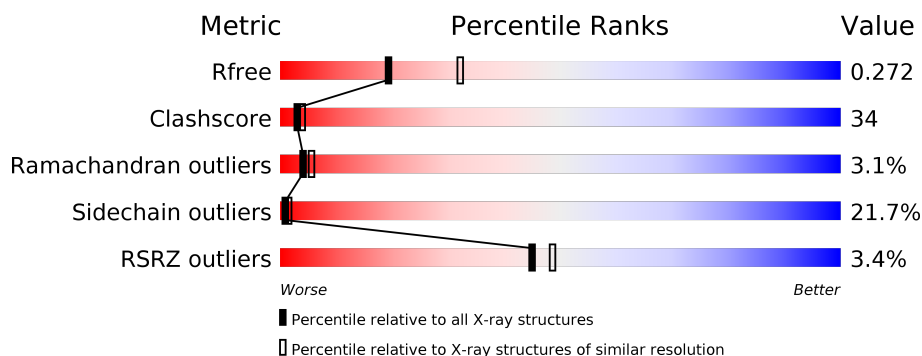
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	301	<div> <div>3%</div> <div> <div></div> <div>43%</div> <div>41%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	301	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>48%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4589 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 Bleomycin acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2242	1406	427	404	5			
1	B	294	Total	C	N	O	S	0	0	0
			2219	1392	421	401	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

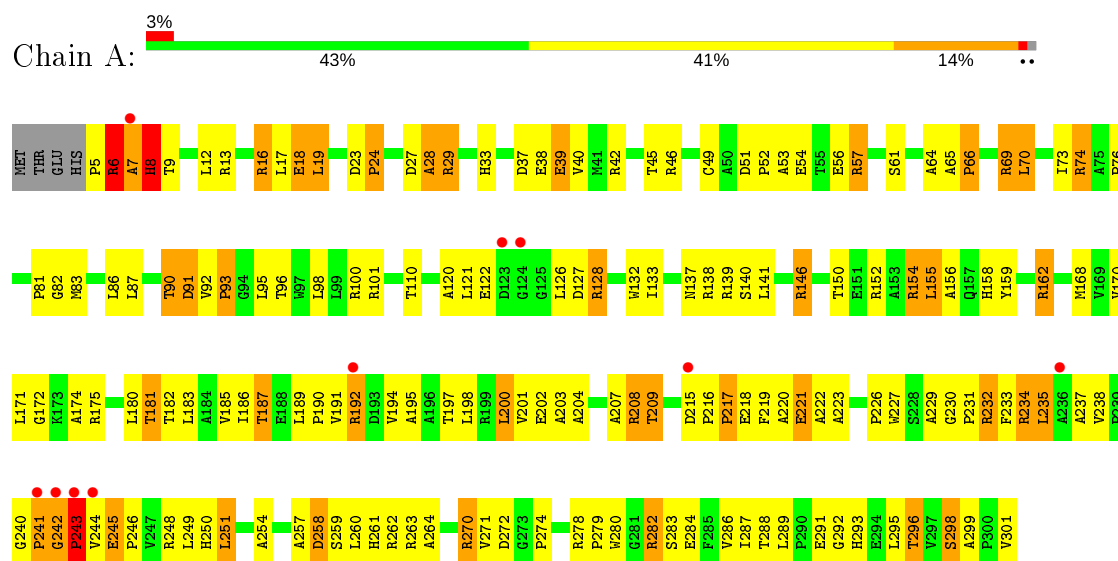
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total 64	O 64	0	0
3	B	44	Total 44	O 44	0	0

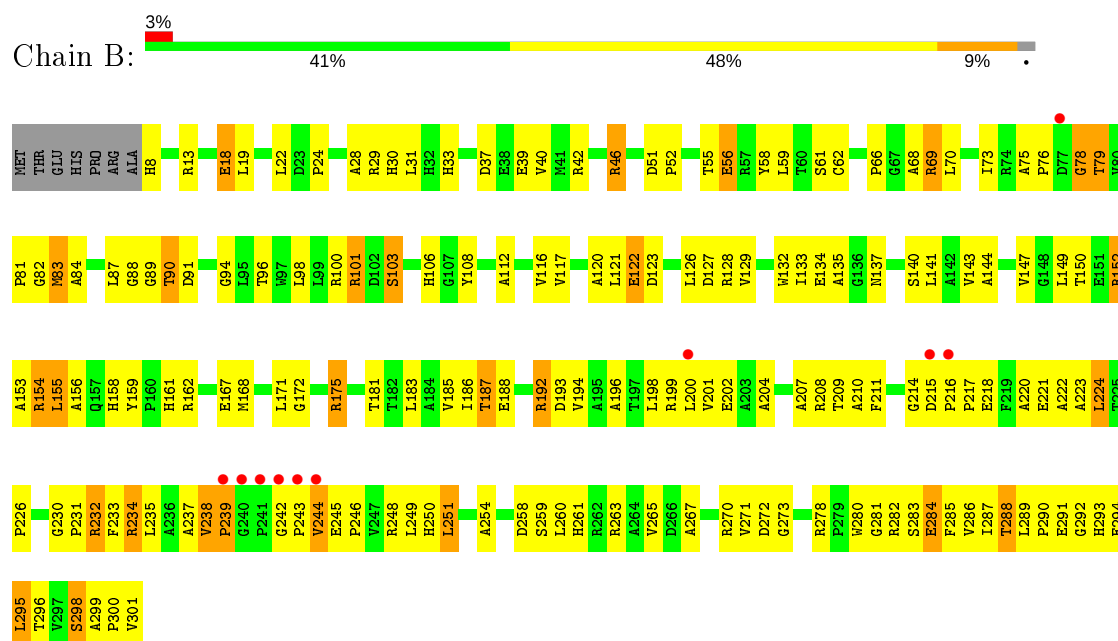
3 Residue-property plots

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

• Molecule 1: Bleomycin acetyltransferase



• Molecule 1: Bleomycin acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.91Å 100.91Å 164.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 48.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.1 (30.00-2.50) 81.6 (48.23-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.272 0.210 , 0.272	Depositor DCC
R_{free} test set	1355 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4589	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: 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	0.33	0/2305	0.64	2/3157 (0.1%)
1	B	0.34	0/2281	0.61	1/3125 (0.0%)
All	All	0.33	0/4586	0.63	3/6282 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	PRO	N-CA-C	6.19	128.19	112.10
1	A	242	GLY	N-CA-C	-6.18	97.64	113.10
1	B	89	GLY	N-CA-C	-5.64	98.99	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2242	0	2211	186	0
1	B	2219	0	2185	147	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
3	A	64	0	0	7	0
3	B	44	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4589	0	4396	303	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 34.

All (303) 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:192:ARG:HH21	1:B:242:GLY:HA2	1.17	1.06
1:A:254:ALA:HB2	1:B:183:LEU:HD11	1.36	1.03
1:A:7:ALA:O	1:A:8:HIS:HB2	1.60	1.00
1:B:87:LEU:HD11	1:B:96:THR:HB	1.51	0.92
1:A:215:ASP:HB3	1:A:216:PRO:HD3	1.50	0.91
1:A:192:ARG:NH1	1:A:243:PRO:HG2	1.84	0.91
1:A:241:PRO:C	1:A:243:PRO:HD3	1.92	0.90
1:B:192:ARG:NH2	1:B:242:GLY:HA2	1.93	0.83
1:B:78:GLY:HA2	3:B:467:HOH:O	1.77	0.83
1:B:201:VAL:HG12	1:B:207:ALA:HB3	1.61	0.82
1:A:221:GLU:HG3	1:A:234:ARG:HH11	1.44	0.81
1:A:198:LEU:HD22	1:A:209:THR:HB	1.63	0.80
1:B:272:ASP:HB2	1:B:286:VAL:HB	1.64	0.80
1:A:8:HIS:O	1:A:9:THR:HG22	1.82	0.79
1:A:87:LEU:HD11	1:A:96:THR:HG23	1.64	0.79
1:A:37:ASP:HB3	1:A:40:VAL:HB	1.65	0.78
1:A:150:THR:O	1:A:152:ARG:HD3	1.83	0.78
1:A:39:GLU:HB2	1:A:101:ARG:HH11	1.50	0.77
1:A:202:GLU:OE1	1:A:209:THR:HG22	1.84	0.76
1:A:180:LEU:HD22	1:B:260:LEU:HG	1.67	0.76
1:A:249:LEU:HB2	1:A:295:LEU:HD22	1.68	0.76
1:A:248:ARG:HB2	1:B:188:GLU:HB3	1.69	0.75
1:A:219:PHE:CZ	1:A:234:ARG:HD2	2.20	0.75
1:B:201:VAL:HG12	1:B:207:ALA:CB	2.17	0.74
1:A:194:VAL:HB	1:A:217:PRO:HB2	1.69	0.73
1:A:250:HIS:HD2	1:B:186:ILE:HD13	1.53	0.73
1:A:201:VAL:HG12	1:A:207:ALA:HB3	1.71	0.73
1:A:257:ALA:HA	1:A:260:LEU:HD12	1.72	0.72
1:B:127:ASP:HA	1:B:175:ARG:HD2	1.71	0.71
1:A:204:ALA:CB	1:A:264:ALA:HA	2.20	0.70
1:B:211:PHE:CZ	1:B:221:GLU:HB2	2.27	0.70
1:A:5:PRO:HB3	1:A:66:PRO:O	1.92	0.69
1:A:12:LEU:HB2	1:A:19:LEU:HB2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:HB1	1:A:264:ALA:HA	1.74	0.68
1:B:127:ASP:O	1:B:175:ARG:HG2	1.93	0.68
1:A:195:ALA:HB2	1:A:217:PRO:HG2	1.76	0.68
1:B:120:ALA:O	1:B:126:LEU:HB2	1.94	0.67
1:B:221:GLU:HG3	1:B:234:ARG:HD3	1.75	0.67
1:B:40:VAL:HG12	1:B:98:LEU:HD11	1.77	0.67
1:B:284:GLU:OE1	1:B:298:SER:HB2	1.95	0.66
1:A:171:LEU:HD12	1:A:171:LEU:H	1.60	0.66
1:B:75:ALA:HB3	1:B:79:THR:HG22	1.78	0.66
1:B:204:ALA:O	1:B:263:ARG:HG2	1.95	0.65
1:A:73:ILE:O	1:A:81:PRO:HD2	1.97	0.65
1:B:147:VAL:O	1:B:147:VAL:HG12	1.98	0.64
1:A:171:LEU:HD12	1:A:171:LEU:N	2.12	0.64
1:A:270:ARG:O	1:A:287:ILE:HA	1.98	0.63
1:A:245:GLU:HB2	1:B:245:GLU:HG2	1.80	0.62
1:B:46:ARG:HD2	1:B:58:TYR:CE1	2.35	0.62
1:A:120:ALA:O	1:A:126:LEU:HB2	2.00	0.62
1:B:83:MET:HG2	1:B:84:ALA:N	2.12	0.62
1:B:221:GLU:OE2	1:B:234:ARG:NH1	2.32	0.62
1:A:39:GLU:CB	1:A:101:ARG:HH11	2.12	0.62
1:A:132:TRP:HB3	1:A:168:MET:HE2	1.81	0.61
1:B:230:GLY:O	1:B:232:ARG:HD2	2.00	0.61
1:A:192:ARG:HD2	1:A:238:VAL:O	2.00	0.61
1:A:219:PHE:HZ	1:A:234:ARG:HD2	1.63	0.61
1:A:241:PRO:O	1:A:243:PRO:HD3	2.01	0.61
1:A:249:LEU:CD2	1:B:187:THR:HB	2.31	0.61
1:A:185:VAL:HG22	1:B:251:LEU:HD12	1.83	0.61
1:B:75:ALA:HB1	1:B:76:PRO:HD2	1.81	0.61
1:A:244:VAL:CG1	1:A:291:GLU:HB3	2.30	0.61
1:B:196:ALA:HA	1:B:199:ARG:NH1	2.14	0.61
1:B:222:ALA:O	1:B:232:ARG:HB2	2.01	0.61
1:A:187:THR:HB	1:B:249:LEU:CD2	2.31	0.61
1:A:180:LEU:HD21	1:B:259:SER:OG	2.00	0.61
1:A:192:ARG:CZ	1:A:243:PRO:HG2	2.31	0.61
1:B:159:TYR:HB2	1:B:162:ARG:CG	2.31	0.60
1:A:286:VAL:HG22	1:A:296:THR:HB	1.81	0.60
1:A:279:PRO:HD2	1:A:280:TRP:CE3	2.37	0.60
1:B:288:THR:HG23	1:B:294:GLU:HB3	1.82	0.59
1:A:198:LEU:HD11	1:A:220:ALA:HB3	1.83	0.59
1:A:254:ALA:HB2	1:B:183:LEU:CD1	2.24	0.59
1:A:284:GLU:HB3	1:A:298:SER:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:CD2	1:A:301:VAL:HG11	2.38	0.59
1:A:185:VAL:HG22	1:B:251:LEU:CD1	2.33	0.59
1:A:132:TRP:HB3	1:A:168:MET:CE	2.33	0.59
1:B:79:THR:HG23	1:B:81:PRO:HD3	1.85	0.59
1:A:16:ARG:O	1:A:76:PRO:HD3	2.04	0.58
1:B:117:VAL:HG21	1:B:147:VAL:HG11	1.86	0.58
1:B:112:ALA:O	1:B:116:VAL:HG23	2.03	0.58
1:B:52:PRO:O	1:B:56:GLU:HB2	2.04	0.58
1:A:70:LEU:N	1:A:70:LEU:HD23	2.19	0.58
1:B:8:HIS:CD2	1:B:69:ARG:HD2	2.39	0.58
1:A:223:ALA:HA	1:A:232:ARG:CB	2.34	0.58
1:B:211:PHE:CE2	1:B:221:GLU:HB2	2.39	0.57
1:A:250:HIS:HB3	1:B:186:ILE:HB	1.86	0.57
1:A:16:ARG:O	1:A:17:LEU:HD23	2.04	0.57
1:A:51:ASP:OD2	1:A:53:ALA:HB3	2.05	0.57
1:A:138:ARG:HD2	3:A:426:HOH:O	2.05	0.57
1:A:215:ASP:HB3	1:A:216:PRO:CD	2.29	0.56
1:B:278:ARG:HD2	1:B:280:TRP:CH2	2.40	0.56
1:A:215:ASP:O	1:A:217:PRO:HD3	2.05	0.56
1:A:249:LEU:HB2	1:A:295:LEU:CD2	2.35	0.56
1:B:87:LEU:HD11	1:B:96:THR:CB	2.29	0.56
1:B:202:GLU:HG3	1:B:207:ALA:O	2.05	0.56
1:A:181:THR:HG22	1:B:254:ALA:HB3	1.87	0.56
1:B:286:VAL:HG12	1:B:287:ILE:N	2.21	0.56
1:B:144:ALA:HB1	1:B:171:LEU:HD22	1.89	0.55
1:B:171:LEU:N	1:B:171:LEU:HD12	2.22	0.55
1:A:221:GLU:HG3	1:A:234:ARG:HD3	1.89	0.55
1:A:244:VAL:HG11	1:A:291:GLU:HB3	1.89	0.55
1:B:37:ASP:HB3	1:B:40:VAL:HG23	1.88	0.55
1:A:39:GLU:HB2	1:A:101:ARG:NH1	2.20	0.55
1:B:242:GLY:H	1:B:243:PRO:HD2	1.72	0.54
1:A:230:GLY:O	1:A:232:ARG:HD2	2.07	0.54
1:A:244:VAL:HG21	1:A:293:HIS:HE1	1.72	0.54
1:A:127:ASP:HB2	3:A:471:HOH:O	2.08	0.54
1:A:87:LEU:HD11	1:A:96:THR:CG2	2.36	0.54
1:A:289:LEU:HD12	1:A:293:HIS:HB2	1.89	0.53
1:B:158:HIS:HE1	1:B:162:ARG:O	1.91	0.53
1:B:193:ASP:HB3	1:B:196:ALA:HB3	1.91	0.53
1:B:134:GLU:OE2	1:B:162:ARG:NH2	2.41	0.53
1:B:132:TRP:C	1:B:168:MET:HE1	2.29	0.53
1:B:137:ASN:O	1:B:141:LEU:HG	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:O	1:B:28:ALA:HB2	2.09	0.53
1:B:75:ALA:HB3	1:B:79:THR:CG2	2.38	0.53
1:A:155:LEU:HD21	1:A:170:VAL:HG21	1.91	0.53
1:A:51:ASP:HB2	1:A:52:PRO:HD2	1.91	0.52
1:B:211:PHE:C	1:B:211:PHE:CD1	2.82	0.52
1:A:159:TYR:HB2	1:A:162:ARG:HG3	1.91	0.52
1:A:194:VAL:HB	1:A:217:PRO:CB	2.37	0.52
1:A:221:GLU:OE2	1:A:234:ARG:NH1	2.42	0.52
1:A:244:VAL:CG2	1:A:245:GLU:N	2.72	0.52
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.24	0.52
1:A:198:LEU:HD11	1:A:220:ALA:CB	2.40	0.52
1:A:246:PRO:HG3	1:A:292:GLY:HA3	1.90	0.52
1:A:90:THR:HG22	1:A:91:ASP:H	1.75	0.52
1:A:110:THR:HG21	1:A:146:ARG:HG2	1.91	0.52
1:A:197:THR:HG21	1:A:235:LEU:HG	1.92	0.52
1:A:174:ALA:HB1	3:A:455:HOH:O	2.09	0.51
1:B:159:TYR:HB2	1:B:162:ARG:HG2	1.93	0.51
1:B:215:ASP:HA	1:B:216:PRO:C	2.29	0.51
1:A:194:VAL:HG23	1:A:237:ALA:HB2	1.92	0.51
1:A:244:VAL:HG22	1:A:245:GLU:N	2.24	0.51
1:B:159:TYR:HB2	1:B:162:ARG:HG3	1.91	0.51
1:B:154:ARG:HD3	1:B:167:GLU:OE1	2.09	0.51
1:A:223:ALA:HA	1:A:232:ARG:HB2	1.93	0.51
1:B:132:TRP:HB3	1:B:168:MET:HE2	1.92	0.51
1:B:210:ALA:HB3	1:B:221:GLU:HB3	1.92	0.51
1:A:250:HIS:CD2	1:B:186:ILE:HD13	2.41	0.51
1:A:242:GLY:N	1:A:243:PRO:HD3	2.24	0.50
1:A:69:ARG:C	1:A:70:LEU:HD23	2.30	0.50
1:B:271:VAL:HG12	1:B:273:GLY:H	1.75	0.50
1:A:221:GLU:CG	1:A:234:ARG:HH11	2.20	0.50
1:A:254:ALA:HB3	1:B:181:THR:HG22	1.92	0.50
1:A:5:PRO:O	1:A:6:ARG:HB2	2.11	0.50
1:A:226:PRO:HD2	1:A:227:TRP:CD1	2.47	0.50
1:A:40:VAL:HG23	1:A:101:ARG:HG2	1.92	0.50
1:A:86:LEU:HD11	1:A:120:ALA:HB2	1.92	0.50
1:B:249:LEU:HB2	1:B:295:LEU:HB3	1.93	0.50
1:B:30:HIS:O	1:B:33:HIS:HB2	2.12	0.50
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.75	0.50
1:A:51:ASP:HB2	1:A:52:PRO:CD	2.42	0.50
1:B:186:ILE:HD12	1:B:186:ILE:N	2.26	0.50
1:A:93:PRO:HG2	1:A:126:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HH11	1:A:29:ARG:CG	2.24	0.50
1:A:229:ALA:HB2	1:B:155:LEU:HD23	1.94	0.50
1:A:223:ALA:HA	1:A:232:ARG:HB3	1.93	0.50
1:A:245:GLU:HA	1:A:245:GLU:OE1	2.11	0.49
1:A:187:THR:HG21	1:A:249:LEU:HD21	1.94	0.49
1:B:272:ASP:HB3	1:B:286:VAL:H	1.77	0.49
1:A:246:PRO:HB3	1:A:292:GLY:O	2.12	0.49
1:A:194:VAL:O	1:A:198:LEU:HD12	2.12	0.49
1:A:96:THR:HG21	3:A:449:HOH:O	2.11	0.49
1:A:191:VAL:HA	1:A:291:GLU:HG2	1.95	0.49
1:B:133:ILE:HD13	1:B:140:SER:HB3	1.94	0.49
1:B:149:LEU:HD23	1:B:172:GLY:C	2.33	0.49
1:A:158:HIS:HA	3:A:427:HOH:O	2.12	0.49
1:A:40:VAL:HG23	1:A:101:ARG:CG	2.42	0.49
1:B:265:VAL:C	1:B:267:ALA:H	2.15	0.49
1:A:13:ARG:HG3	1:A:18:GLU:HG2	1.94	0.48
1:B:198:LEU:HD11	1:B:220:ALA:CB	2.43	0.48
1:B:55:THR:HG22	1:B:59:LEU:CD1	2.43	0.48
1:A:257:ALA:HB2	1:A:299:ALA:HB3	1.94	0.48
1:A:254:ALA:CB	1:B:183:LEU:HD11	2.26	0.48
1:A:137:ASN:O	1:A:141:LEU:HD12	2.13	0.48
1:B:280:TRP:CD1	1:B:282:ARG:HB2	2.49	0.48
1:B:286:VAL:CG1	1:B:287:ILE:N	2.76	0.48
1:B:68:ALA:O	1:B:69:ARG:HD3	2.13	0.48
1:A:284:GLU:OE1	1:A:298:SER:HB2	2.14	0.48
1:B:143:VAL:O	1:B:147:VAL:HG23	2.14	0.48
1:B:246:PRO:HB3	1:B:292:GLY:O	2.13	0.48
1:A:137:ASN:CG	1:A:140:SER:HB2	2.34	0.48
1:A:200:LEU:O	1:A:203:ALA:HB3	2.14	0.48
1:B:156:ALA:HB1	1:B:300:PRO:HG3	1.96	0.48
1:B:73:ILE:CG2	1:B:81:PRO:HG2	2.44	0.48
1:B:13:ARG:HG3	1:B:18:GLU:OE1	2.14	0.47
1:A:183:LEU:HD11	1:B:254:ALA:HB2	1.95	0.47
1:B:39:GLU:OE1	1:B:101:ARG:HD2	2.14	0.47
1:B:150:THR:O	1:B:152:ARG:HD3	2.14	0.47
1:B:244:VAL:HG11	1:B:291:GLU:HB2	1.96	0.47
1:A:282:ARG:HH11	1:A:282:ARG:HG2	1.80	0.47
1:A:249:LEU:HD21	1:B:187:THR:HB	1.96	0.47
1:A:49:CYS:HB3	1:A:54:GLU:HB3	1.95	0.47
1:B:155:LEU:HD12	1:B:168:MET:HB2	1.97	0.47
1:A:74:ARG:CG	1:A:74:ARG:HH11	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ALA:HA	1:B:199:ARG:CZ	2.45	0.46
1:B:210:ALA:O	1:B:211:PHE:HB3	2.16	0.46
1:A:286:VAL:HG22	1:A:296:THR:CB	2.44	0.46
1:B:198:LEU:HD22	1:B:209:THR:OG1	2.15	0.46
1:A:208:ARG:HH11	1:A:226:PRO:HA	1.81	0.46
1:A:215:ASP:CB	1:A:216:PRO:HD3	2.35	0.46
1:A:242:GLY:N	1:A:243:PRO:CD	2.79	0.46
1:B:73:ILE:HD12	1:B:83:MET:N	2.30	0.46
1:A:154:ARG:HB3	1:B:183:LEU:HD23	1.97	0.46
1:B:159:TYR:HB3	1:B:161:HIS:CD2	2.50	0.45
1:B:73:ILE:HD12	1:B:82:GLY:C	2.36	0.45
1:A:186:ILE:HG23	1:A:233:PHE:HA	1.98	0.45
1:A:204:ALA:O	1:A:263:ARG:NE	2.49	0.45
1:A:271:VAL:HA	1:A:286:VAL:O	2.17	0.45
1:A:282:ARG:CG	1:A:282:ARG:HH11	2.30	0.45
1:A:246:PRO:HB3	1:A:292:GLY:C	2.36	0.45
1:A:6:ARG:HD2	1:A:6:ARG:HA	1.49	0.45
1:A:137:ASN:OD1	1:A:140:SER:HB2	2.16	0.45
1:A:152:ARG:NH1	1:A:172:GLY:O	2.49	0.45
1:B:135:ALA:HB2	1:B:167:GLU:HB3	1.98	0.45
1:B:299:ALA:HB1	1:B:300:PRO:HD2	1.99	0.45
1:A:189:LEU:HB2	1:A:235:LEU:HD12	1.97	0.45
1:A:271:VAL:O	1:A:271:VAL:HG23	2.15	0.45
1:A:286:VAL:HA	1:A:296:THR:HA	1.98	0.45
1:B:214:GLY:O	1:B:217:PRO:HA	2.16	0.45
1:B:242:GLY:N	1:B:243:PRO:CD	2.80	0.45
1:B:289:LEU:HD12	1:B:293:HIS:HB2	1.98	0.45
1:A:289:LEU:HD12	1:A:293:HIS:CD2	2.51	0.45
1:A:8:HIS:NE2	1:A:69:ARG:HG3	2.32	0.45
1:A:198:LEU:HG	1:A:235:LEU:HD23	1.98	0.45
1:A:238:VAL:HG23	1:A:238:VAL:O	2.16	0.45
1:B:134:GLU:HA	1:B:168:MET:SD	2.57	0.45
1:B:161:HIS:CD2	1:B:161:HIS:H	2.34	0.45
1:A:156:ALA:O	1:A:282:ARG:NH2	2.50	0.44
1:A:291:GLU:OE1	1:A:291:GLU:N	2.46	0.44
1:B:223:ALA:HA	1:B:232:ARG:CB	2.47	0.44
1:A:127:ASP:HB3	1:A:128:ARG:NH1	2.32	0.44
1:B:144:ALA:CB	1:B:171:LEU:HD22	2.48	0.44
1:A:181:THR:HG22	1:B:254:ALA:CB	2.48	0.44
1:A:229:ALA:HB3	1:B:153:ALA:HB3	1.99	0.44
1:A:181:THR:HG23	1:A:182:THR:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:O	1:A:232:ARG:HB3	2.18	0.44
1:A:180:LEU:CD2	1:B:260:LEU:HG	2.44	0.44
1:A:100:ARG:HB2	3:A:429:HOH:O	2.16	0.44
1:B:187:THR:O	1:B:233:PHE:HB2	2.18	0.44
1:A:237:ALA:O	1:A:238:VAL:HG13	2.18	0.43
1:A:190:PRO:HG2	1:A:244:VAL:HG21	2.00	0.43
1:A:261:HIS:CE1	1:A:274:PRO:HA	2.53	0.43
1:A:57:ARG:NH2	2:A:404:SO4:O1	2.51	0.43
1:B:58:TYR:CE2	1:B:62:CYS:SG	3.09	0.43
1:B:88:GLY:C	1:B:90:THR:H	2.21	0.43
1:A:192:ARG:NH2	1:A:240:GLY:O	2.51	0.43
1:B:223:ALA:HA	1:B:232:ARG:HB2	2.00	0.43
1:A:249:LEU:HD23	1:B:187:THR:HB	2.01	0.43
1:B:261:HIS:HA	1:B:285:PHE:CZ	2.54	0.43
1:B:122:GLU:HB3	1:B:123:ASP:H	1.59	0.43
1:A:29:ARG:NH1	1:A:29:ARG:CG	2.82	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.84	0.43
1:A:6:ARG:HB3	1:A:7:ALA:H	1.33	0.43
1:B:186:ILE:HG22	1:B:234:ARG:HG2	2.01	0.43
1:A:186:ILE:HD12	1:A:186:ILE:N	2.33	0.43
1:B:281:GLY:O	1:B:282:ARG:HG2	2.19	0.43
1:A:278:ARG:HB3	1:A:279:PRO:CD	2.49	0.42
1:B:158:HIS:CD2	1:B:301:VAL:HG11	2.55	0.42
1:A:64:ALA:O	1:A:65:ALA:C	2.57	0.42
1:A:8:HIS:HB3	1:A:9:THR:H	1.17	0.42
1:B:103:SER:HB3	1:B:108:TYR:CD2	2.55	0.42
1:A:244:VAL:O	1:A:246:PRO:HD3	2.20	0.42
1:B:19:LEU:CD2	1:B:73:ILE:HA	2.50	0.42
1:B:208:ARG:HE	1:B:226:PRO:HA	1.85	0.42
1:A:45:THR:HA	1:A:159:TYR:CE2	2.55	0.42
1:A:128:ARG:HB3	1:A:128:ARG:CZ	2.49	0.42
1:A:46:ARG:NH2	1:A:54:GLU:OE1	2.50	0.42
1:B:149:LEU:O	1:B:171:LEU:HD23	2.20	0.42
1:A:183:LEU:HD22	1:B:155:LEU:HA	2.01	0.42
1:A:186:ILE:HG23	1:A:232:ARG:O	2.19	0.42
1:A:251:LEU:CD1	1:B:185:VAL:HG22	2.50	0.41
1:B:194:VAL:HG23	1:B:237:ALA:HB2	2.01	0.41
1:B:94:GLY:HA3	3:B:428:HOH:O	2.20	0.41
1:A:258:ASP:OD1	1:A:262:ARG:NH2	2.54	0.41
1:B:147:VAL:CG1	1:B:147:VAL:O	2.66	0.41
1:B:224:LEU:HD12	1:B:231:PRO:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLU:H	1:B:291:GLU:CD	2.24	0.41
1:A:82:GLY:HA3	1:A:98:LEU:O	2.20	0.41
1:A:229:ALA:HB3	1:B:153:ALA:CB	2.51	0.41
1:A:258:ASP:OD2	1:A:259:SER:N	2.54	0.41
1:A:154:ARG:NE	3:A:430:HOH:O	2.53	0.41
1:A:201:VAL:CG1	1:A:207:ALA:HB3	2.46	0.41
1:B:132:TRP:N	1:B:132:TRP:CD1	2.88	0.41
1:B:117:VAL:HG21	1:B:147:VAL:CG1	2.51	0.41
1:B:238:VAL:HA	1:B:239:PRO:HD3	1.92	0.41
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.85	0.41
1:B:73:ILE:HG22	1:B:81:PRO:HG2	2.03	0.41
1:A:200:LEU:O	1:A:203:ALA:N	2.54	0.41
1:B:193:ASP:OD1	1:B:196:ALA:HB2	2.20	0.41
1:A:23:ASP:O	1:A:24:PRO:C	2.59	0.41
1:A:33:HIS:CD2	1:A:100:ARG:NH2	2.89	0.41
1:B:144:ALA:O	1:B:149:LEU:HB2	2.21	0.41
1:A:234:ARG:NH2	1:B:250:HIS:CD2	2.89	0.41
1:A:249:LEU:HD23	1:B:187:THR:HA	2.01	0.40
1:A:187:THR:HG21	1:B:187:THR:HB	2.02	0.40
1:A:222:ALA:O	1:A:232:ARG:HB2	2.21	0.40
1:A:27:ASP:O	1:A:28:ALA:C	2.60	0.40
1:A:250:HIS:CE1	1:A:298:SER:HB3	2.56	0.40
1:B:287:ILE:O	1:B:294:GLU:HA	2.20	0.40
1:A:289:LEU:HD12	1:A:293:HIS:HD2	1.87	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	295/301 (98%)	256 (87%)	28 (10%)	11 (4%)	3 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	292/301 (97%)	258 (88%)	27 (9%)	7 (2%)	6	9
All	All	587/602 (98%)	514 (88%)	55 (9%)	18 (3%)	4	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	ALA
1	A	8	HIS
1	A	66	PRO
1	A	241	PRO
1	B	244	VAL
1	B	66	PRO
1	B	122	GLU
1	A	24	PRO
1	A	243	PRO
1	B	239	PRO
1	A	28	ALA
1	A	93	PRO
1	A	217	PRO
1	A	272	ASP
1	B	78	GLY
1	B	290	PRO
1	B	79	THR

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	218/222 (98%)	167 (77%)	51 (23%)	1	1
1	B	216/222 (97%)	173 (80%)	43 (20%)	1	2
All	All	434/444 (98%)	340 (78%)	94 (22%)	1	1

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	HIS
1	A	16	ARG
1	A	18	GLU
1	A	19	LEU
1	A	29	ARG
1	A	38	GLU
1	A	39	GLU
1	A	42	ARG
1	A	56	GLU
1	A	57	ARG
1	A	61	SER
1	A	69	ARG
1	A	70	LEU
1	A	74	ARG
1	A	83	MET
1	A	90	THR
1	A	91	ASP
1	A	92	VAL
1	A	95	LEU
1	A	121	LEU
1	A	122	GLU
1	A	128	ARG
1	A	133	ILE
1	A	139	ARG
1	A	146	ARG
1	A	154	ARG
1	A	155	LEU
1	A	162	ARG
1	A	175	ARG
1	A	181	THR
1	A	187	THR
1	A	192	ARG
1	A	200	LEU
1	A	208	ARG
1	A	209	THR
1	A	218	GLU
1	A	221	GLU
1	A	232	ARG
1	A	234	ARG
1	A	235	LEU
1	A	243	PRO
1	A	245	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	251	LEU
1	A	258	ASP
1	A	270	ARG
1	A	282	ARG
1	A	283	SER
1	A	288	THR
1	A	296	THR
1	A	298	SER
1	B	18	GLU
1	B	22	LEU
1	B	29	ARG
1	B	42	ARG
1	B	46	ARG
1	B	51	ASP
1	B	56	GLU
1	B	61	SER
1	B	69	ARG
1	B	70	LEU
1	B	83	MET
1	B	90	THR
1	B	91	ASP
1	B	100	ARG
1	B	101	ARG
1	B	103	SER
1	B	106	HIS
1	B	121	LEU
1	B	128	ARG
1	B	129	VAL
1	B	152	ARG
1	B	154	ARG
1	B	155	LEU
1	B	175	ARG
1	B	187	THR
1	B	192	ARG
1	B	200	LEU
1	B	218	GLU
1	B	224	LEU
1	B	232	ARG
1	B	234	ARG
1	B	235	LEU
1	B	238	VAL
1	B	248	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	251	LEU
1	B	258	ASP
1	B	270	ARG
1	B	283	SER
1	B	284	GLU
1	B	288	THR
1	B	295	LEU
1	B	296	THR
1	B	298	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	261	HIS
1	B	8	HIS
1	B	11	HIS
1	B	157	GLN
1	B	158	HIS
1	B	161	HIS
1	B	250	HIS
1	B	261	HIS

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	404	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	A	402	-	4,4,4	0.28	0	6,6,6	0.13	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	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, 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	297/301 (98%)	-0.20	10 (3%) 45 48	13, 39, 86, 100	0
1	B	294/301 (97%)	-0.13	10 (3%) 45 48	11, 43, 83, 100	0
All	All	591/602 (98%)	-0.16	20 (3%) 45 48	11, 41, 85, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	GLY	4.5
1	B	241	PRO	4.4
1	A	241	PRO	4.1
1	B	242	GLY	4.0
1	A	243	PRO	3.3
1	A	7	ALA	3.1
1	B	239	PRO	2.9
1	B	243	PRO	2.8
1	A	244	VAL	2.8
1	A	192	ARG	2.7
1	B	77	ASP	2.6
1	B	215	ASP	2.4
1	B	200	LEU	2.4
1	A	123	ASP	2.4
1	A	236	ALA	2.3
1	B	240	GLY	2.3
1	B	216	PRO	2.2
1	A	215	ASP	2.2
1	A	242	GLY	2.2
1	B	244	VAL	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. 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(\AA^2)	Q<0.9
2	SO4	A	404	5/5	0.95	0.14	48,62,67,69	0
2	SO4	B	403	5/5	0.96	0.14	41,63,65,68	0
2	SO4	A	402	5/5	0.97	0.13	54,71,74,74	0
2	SO4	A	401	5/5	0.99	0.13	18,20,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.