



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 11:43 pm BST

PDB ID : 2UVE / pdb\_00002uve  
Title : Structure of Yersinia enterocolitica Family 28 Exopolygalacturonase  
Authors : Abbott, D.W.; Boraston, A.B.  
Deposited on : 2007-03-09  
Resolution : 2.19 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

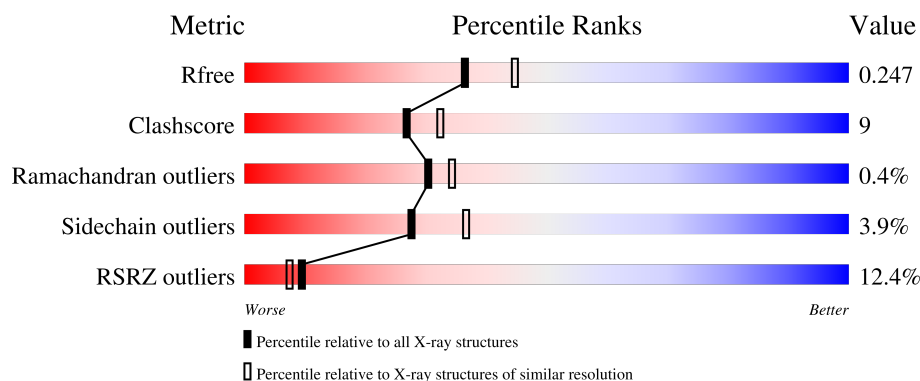
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	608	 13% 75% 16% • 6%
1	B	608	 11% 77% 13% • 7%

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	1616	-	-	X	-
3	SO4	B	1619	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9409 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.

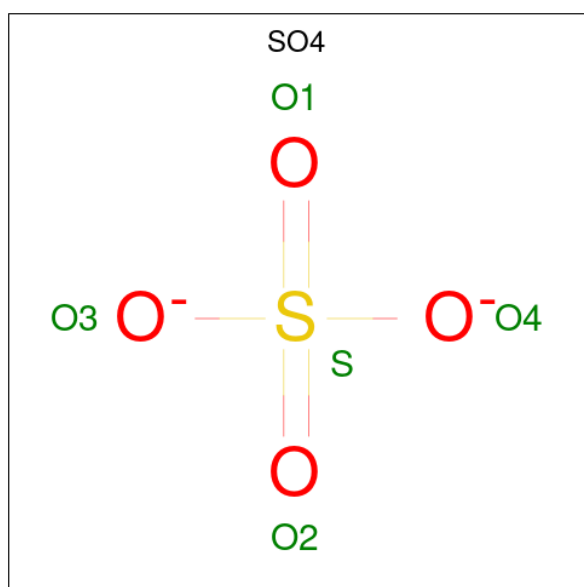
- Molecule 1 is a protein called EXOPOLYGALACTURONASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	2	0
			4439	2784	776	864	15			
1	B	566	Total	C	N	O	S	0	1	0
			4399	2764	769	851	15			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ni	0	0
			4	4		
2	B	5	Total	Ni	0	0
			5	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

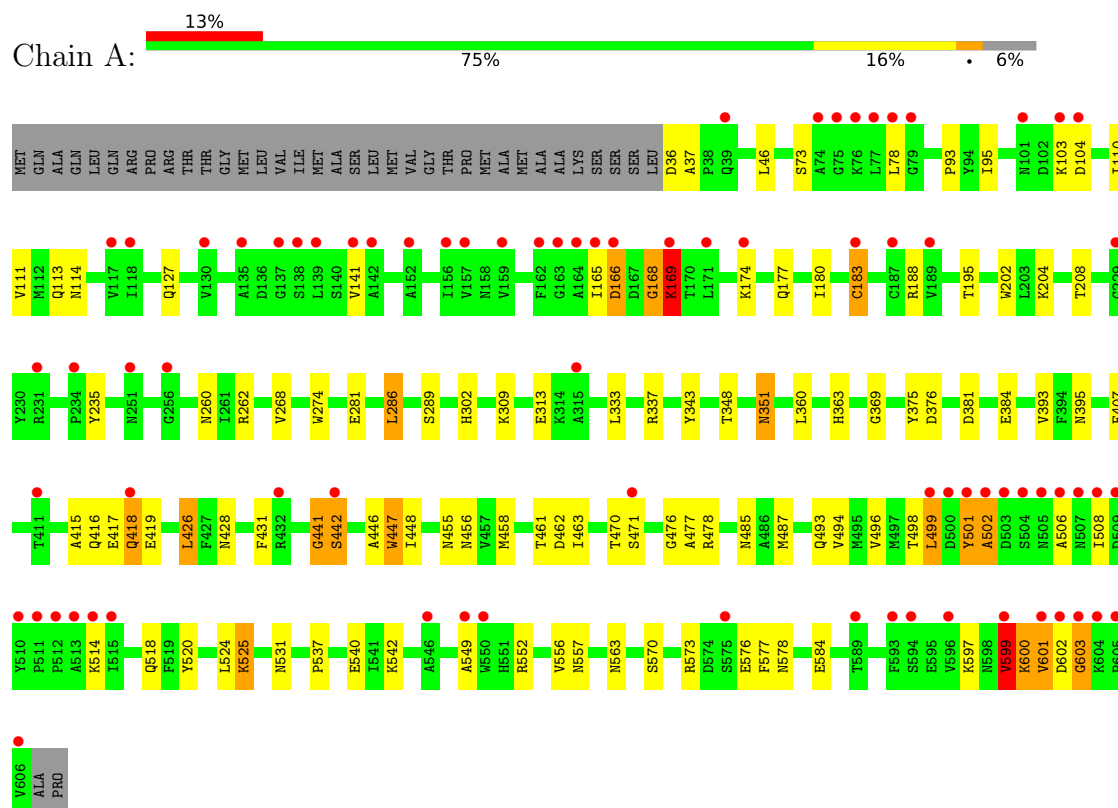
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	286	Total	O	0	0
			286	286		

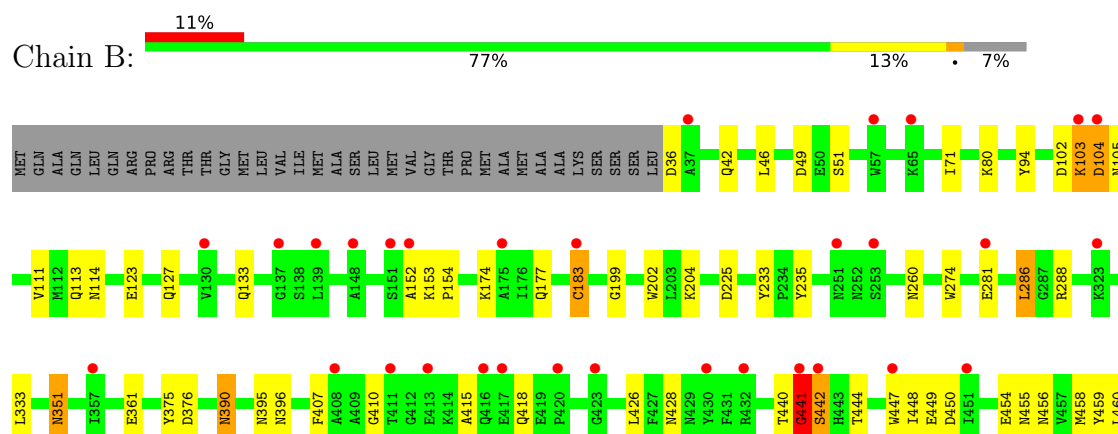
### 3 Residue-property plots

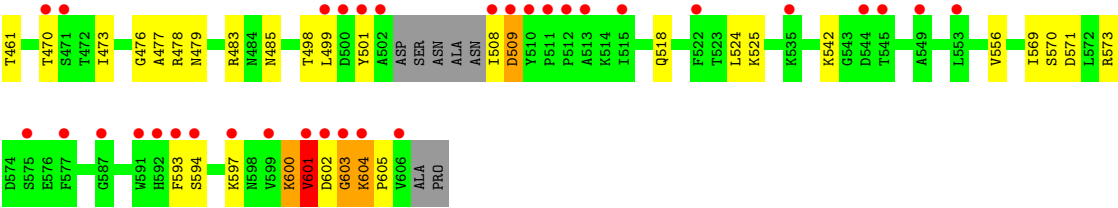
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: EXOPOLYGALACTURONASE



#### • Molecule 1: EXOPOLYGALACTURONASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.95Å 78.76Å 98.19Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	34.42 – 2.19 34.42 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-2.19) 99.9 (34.42-2.19)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.228 0.246 , 0.247	Depositor DCC
$R_{free}$ test set	3467 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: ACT, SO4, NI

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	0.85	1/4532 (0.0%)	0.82	2/6153 (0.0%)
1	B	0.94	1/4491 (0.0%)	0.86	5/6094 (0.1%)
All	All	0.90	2/9023 (0.0%)	0.84	7/12247 (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	A	0	8
1	B	0	7
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	CYS	CB-SG	-8.56	1.67	1.82
1	A	183	CYS	CB-SG	-7.20	1.70	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	601	VAL	N-CA-C	8.21	133.16	111.00
1	B	442	SER	N-CA-CB	6.96	120.93	110.50
1	A	188	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	441	GLY	C-N-CA	6.09	136.93	121.70
1	B	49	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	603	GLY	CA-C-O	-5.21	111.22	120.60
1	A	462	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLY	Peptide
1	A	441	GLY	Peptide
1	A	501	TYR	Peptide
1	A	502	ALA	Peptide
1	A	599	VAL	Peptide
1	A	600	LYS	Mainchain
1	A	601	VAL	Peptide
1	A	603	GLY	Peptide
1	B	102	ASP	Peptide
1	B	440	THR	Peptide
1	B	441	GLY	Peptide
1	B	501	TYR	Peptide
1	B	600	LYS	Peptide
1	B	601	VAL	Peptide
1	B	604	LYS	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	4439	0	4323	83	0
1	B	4399	0	4298	70	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	55	0	0	6	0
3	B	40	0	0	4	0
4	B	4	0	3	0	0
5	A	177	0	0	5	0
5	B	286	0	0	9	0
All	All	9409	0	8624	157	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 9.

All (157) 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:604:LYS:HB3	1:B:605:PRO:HD3	1.27	1.16
1:A:602:ASP:N	1:A:603:GLY:HA2	1.72	1.05
1:B:603:GLY:O	1:B:604:LYS:CG	2.05	1.04
1:B:604:LYS:CB	1:B:605:PRO:HD3	1.89	1.01
1:A:415:ALA:O	1:A:418:GLN:HG3	1.61	1.00
1:B:603:GLY:O	1:B:604:LYS:HG2	1.66	0.93
1:A:313:GLU:HG3	5:A:2094:HOH:O	1.67	0.91
3:A:1619:SO4:O1	5:A:2176:HOH:O	1.89	0.90
1:A:601:VAL:HG12	1:A:602:ASP:HB3	1.53	0.90
1:B:407:PHE:O	1:B:441:GLY:HA3	1.72	0.89
1:B:603:GLY:O	1:B:604:LYS:HG3	1.71	0.88
1:B:113:GLN:H	1:B:428:ASN:HD21	1.15	0.88
1:A:602:ASP:H	1:A:603:GLY:HA2	1.40	0.86
1:B:450:ASP:OD1	1:B:479:ASN:ND2	2.09	0.85
1:A:113:GLN:H	1:A:428:ASN:HD21	1.24	0.85
1:B:602:ASP:N	1:B:603:GLY:HA2	1.94	0.81
3:B:1619:SO4:S	5:B:2285:HOH:O	2.37	0.81
1:A:418:GLN:OE1	5:A:2135:HOH:O	1.99	0.80
1:A:37:ALA:HB2	1:A:141:VAL:HG23	1.63	0.80
1:B:177:GLN:HE22	1:B:202:TRP:H	1.29	0.80
1:B:600:LYS:NZ	1:B:604:LYS:HE2	1.97	0.79
1:A:599:VAL:HG23	1:A:600:LYS:H	1.48	0.79
1:A:177:GLN:HE22	1:A:202:TRP:H	1.29	0.78
1:A:531[A]:ASN:HD22	1:A:563[A]:ASN:HB3	1.49	0.76
1:B:604:LYS:HB3	1:B:605:PRO:CD	2.14	0.75
1:A:577:PHE:O	1:A:602:ASP:HB2	1.86	0.75
1:A:602:ASP:N	1:A:603:GLY:CA	2.50	0.74
1:B:415:ALA:HA	1:B:418:GLN:HE21	1.51	0.74
1:A:600:LYS:HE2	3:A:1616:SO4:O2	1.87	0.74
1:A:506:ALA:HB1	1:A:508:ILE:HG12	1.68	0.73
1:A:281:GLU:OE1	1:A:289:SER:HB2	1.90	0.72
1:B:601:VAL:HG23	1:B:602:ASP:HB3	1.71	0.72
1:A:600:LYS:HD3	3:A:1616:SO4:O2	1.90	0.71
3:B:1619:SO4:O2	5:B:2285:HOH:O	2.07	0.71
1:B:288[A]:ARG:NH1	5:B:2157:HOH:O	2.06	0.69
1:A:168:GLY:O	1:A:169:LYS:HB3	1.92	0.69
1:A:600:LYS:CE	3:A:1616:SO4:O2	2.41	0.68
1:A:456:ASN:H	1:A:485:ASN:HD22	1.40	0.67
1:A:499:LEU:HD13	1:A:549:ALA:HB1	1.77	0.67
1:B:456:ASN:H	1:B:485:ASN:HD22	1.44	0.66
1:B:274:TRP:H	1:B:351:ASN:HD21	1.42	0.66
1:A:113:GLN:N	1:A:428:ASN:HD21	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LYS:HZ2	1:B:604:LYS:HE2	1.59	0.66
3:B:1613:SO4:O3	5:B:2282:HOH:O	2.10	0.65
1:B:183:CYS:HB2	1:B:204:LYS:HE2	1.78	0.65
1:B:361:GLU:HG3	5:B:2190:HOH:O	1.94	0.65
1:A:363:HIS:NE2	1:A:419:GLU:OE1	2.21	0.65
1:B:600:LYS:HD3	1:B:604:LYS:HG2	1.79	0.64
1:A:601:VAL:CG1	1:A:602:ASP:HB3	2.26	0.63
1:B:604:LYS:CB	1:B:605:PRO:CD	2.71	0.62
1:A:166:ASP:HB2	1:A:195:THR:O	1.99	0.62
1:B:508:ILE:N	5:B:2245:HOH:O	2.32	0.62
1:A:602:ASP:O	1:A:602:ASP:CG	2.37	0.61
1:A:578:ASN:HA	1:A:602:ASP:HB2	1.83	0.61
1:A:442:SER:CB	3:A:1621:SO4:O4	2.49	0.60
1:A:268:VAL:HG22	1:A:348:THR:HB	1.84	0.60
1:B:113:GLN:N	1:B:428:ASN:HD21	1.95	0.59
1:B:603:GLY:C	1:B:604:LYS:CG	2.70	0.58
1:A:599:VAL:HG23	1:A:600:LYS:N	2.15	0.58
1:A:600:LYS:CD	3:A:1616:SO4:O2	2.51	0.58
1:A:73:SER:HB2	1:A:78:LEU:HD11	1.87	0.57
1:A:113:GLN:H	1:A:428:ASN:ND2	1.98	0.57
1:B:603:GLY:C	1:B:604:LYS:HG3	2.24	0.57
1:B:235:TYR:OH	1:B:418:GLN:NE2	2.40	0.55
1:A:531[A]:ASN:ND2	1:A:563[A]:ASN:HB3	2.21	0.55
1:A:576:GLU:HA	1:A:600:LYS:O	2.07	0.55
1:A:103:LYS:O	1:A:104:ASP:HB2	2.07	0.54
1:A:501:TYR:CD2	1:A:502:ALA:HA	2.42	0.54
1:B:390:ASN:HB2	5:B:2208:HOH:O	2.07	0.54
1:A:302:HIS:O	1:A:309:LYS:HE3	2.08	0.54
1:B:114:ASN:HD21	1:B:395:ASN:HD21	1.57	0.53
1:A:337:ARG:HA	1:A:360:LEU:O	2.09	0.53
1:B:600:LYS:HZ3	1:B:604:LYS:HE2	1.73	0.53
1:B:274:TRP:N	1:B:351:ASN:HD21	2.07	0.52
1:A:93:PRO:HB2	1:A:286:LEU:HD21	1.92	0.52
1:A:416:GLN:C	1:A:418:GLN:H	2.13	0.52
1:A:563[A]:ASN:HA	1:A:584:GLU:O	2.09	0.52
1:A:506:ALA:HB1	1:A:508:ILE:CG1	2.40	0.52
1:A:183:CYS:HB2	1:A:204:LYS:HE2	1.92	0.51
1:A:446:ALA:O	1:A:447:TRP:HB2	2.11	0.51
1:B:602:ASP:N	1:B:603:GLY:CA	2.72	0.51
1:B:454:GLU:HA	1:B:483:ARG:O	2.11	0.50
1:B:570:SER:HA	1:B:594:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HB2	1:A:540:GLU:HB2	1.94	0.50
1:B:103:LYS:HG3	1:B:104:ASP:HA	1.93	0.50
1:B:113:GLN:H	1:B:428:ASN:ND2	1.97	0.50
1:A:573:ARG:HA	1:A:597:LYS:O	2.13	0.49
1:B:470:THR:OG1	1:B:473:ILE:HG12	2.12	0.49
1:B:390:ASN:ND2	5:B:2208:HOH:O	2.45	0.49
1:A:114:ASN:HD21	1:A:395:ASN:HD21	1.61	0.49
1:A:525:LYS:HG3	1:A:557:ASN:HB2	1.95	0.49
1:B:508:ILE:HA	1:B:509:ASP:HA	1.42	0.48
1:B:51:SER:HB3	5:B:2068:HOH:O	2.12	0.48
1:B:199:GLY:HA3	1:B:225:ASP:HB3	1.94	0.48
1:A:456:ASN:H	1:A:485:ASN:ND2	2.10	0.48
1:A:46:LEU:HD11	1:A:260:ASN:HA	1.96	0.47
1:A:496:VAL:HG12	1:A:498:THR:HG23	1.96	0.47
1:A:578:ASN:OD1	1:A:602:ASP:HA	2.13	0.47
1:A:281:GLU:OE1	1:A:289:SER:CB	2.61	0.47
1:A:407:PHE:O	1:A:441:GLY:HA3	2.13	0.47
1:A:599:VAL:CG2	1:A:600:LYS:N	2.78	0.47
1:A:499:LEU:HD12	5:A:2160:HOH:O	2.14	0.47
1:B:483:ARG:HA	1:B:525:LYS:O	2.15	0.47
1:A:274:TRP:H	1:A:351:ASN:HD21	1.62	0.47
1:A:111:VAL:H	1:A:455:ASN:ND2	2.13	0.46
1:A:487:MET:HE3	1:A:494:VAL:HG13	1.97	0.46
1:A:463:ILE:HA	1:A:493:GLN:O	2.15	0.46
1:B:602:ASP:H	1:B:603:GLY:HA2	1.78	0.46
1:A:478:ARG:HA	1:A:520:TYR:O	2.16	0.46
1:A:262:ARG:HG2	1:A:343:TYR:HB3	1.98	0.45
1:B:111:VAL:H	1:B:455:ASN:ND2	2.13	0.45
1:B:448:ILE:O	1:B:477:ALA:HA	2.16	0.45
1:B:524:LEU:O	1:B:556:VAL:HA	2.17	0.45
1:B:80:LYS:HE3	1:B:133:GLN:OE1	2.17	0.45
1:B:103:LYS:CG	1:B:104:ASP:HA	2.47	0.45
1:B:602:ASP:O	1:B:602:ASP:CG	2.50	0.44
1:B:498:THR:HG22	1:B:542:LYS:HD3	1.99	0.44
1:B:114:ASN:ND2	1:B:395:ASN:HD21	2.16	0.44
1:B:573:ARG:HA	1:B:597:LYS:O	2.16	0.44
1:A:180:ILE:O	1:A:183:CYS:HB2	2.18	0.44
1:A:501:TYR:CG	1:A:502:ALA:HA	2.52	0.44
1:A:524:LEU:HB3	1:A:556:VAL:HG22	1.99	0.44
1:B:459:TYR:O	1:B:460:LEU:HB2	2.17	0.44
1:B:94:TYR:CD1	1:B:286:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HA	1:B:105:ASN:H	1.82	0.43
1:A:552:ARG:HA	1:A:573:ARG:O	2.19	0.43
1:B:444:THR:H	1:B:473:ILE:HG21	1.84	0.43
1:B:42:GLN:NE2	3:B:1616:SO4:O4	2.51	0.43
1:B:600:LYS:HB3	1:B:604:LYS:HA	2.01	0.43
1:B:71:ILE:HD12	1:B:71:ILE:N	2.33	0.43
1:A:476:GLY:HA3	1:A:518:GLN:O	2.19	0.43
1:A:573:ARG:HD3	1:A:597:LYS:HB3	2.00	0.43
1:A:235:TYR:OH	1:A:418:GLN:NE2	2.53	0.42
1:A:448:ILE:O	1:A:477:ALA:HA	2.19	0.42
1:A:416:GLN:C	1:A:418:GLN:N	2.73	0.42
1:A:114:ASN:ND2	1:A:395:ASN:HD21	2.17	0.42
1:B:569:ILE:O	1:B:593:PHE:HA	2.20	0.42
1:A:114:ASN:ND2	5:A:2030:HOH:O	2.51	0.42
1:B:274:TRP:H	1:B:351:ASN:ND2	2.12	0.41
1:B:46:LEU:HD11	1:B:260:ASN:HA	2.02	0.41
1:B:449:GLU:HA	1:B:478:ARG:O	2.20	0.41
1:A:563[B]:ASN:HA	1:A:584:GLU:O	2.19	0.41
1:B:600:LYS:HZ3	1:B:604:LYS:CE	2.32	0.41
1:B:103:LYS:CB	1:B:104:ASP:HA	2.50	0.41
1:B:233:TYR:CZ	1:B:410:GLY:HA2	2.56	0.41
1:B:375:TYR:HA	1:B:376:ASP:HA	1.84	0.41
1:A:369:GLY:HA2	1:A:395:ASN:O	2.20	0.40
1:A:375:TYR:HA	1:A:376:ASP:HA	1.79	0.40
1:A:381:ASP:OD2	1:A:384:GLU:OE2	2.39	0.40
1:A:431:PHE:HB2	1:A:458:MET:HG3	2.02	0.40
1:A:95:ILE:HG21	1:A:110:ILE:HD11	2.04	0.40
1:A:542:LYS:HA	1:A:570:SER:HB2	2.03	0.40
1:B:476:GLY:HA3	1:B:518:GLN:O	2.21	0.40
1:A:208:THR:HA	1:A:262:ARG:O	2.21	0.40
1:A:393:VAL:HB	1:A:426:LEU:HD12	2.02	0.40
1:B:123:GLU:HG3	1:B:152:ALA:HA	2.04	0.40
1:B:153:LYS:HD2	1:B:154:PRO:HD2	2.02	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	571/608 (94%)	526 (92%)	42 (7%)	3 (0%)	25	28
1	B	563/608 (93%)	526 (93%)	35 (6%)	2 (0%)	30	34
All	All	1134/1216 (93%)	1052 (93%)	77 (7%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	SER
1	A	169	LYS
1	A	417	GLU
1	B	447	TRP
1	A	447	TRP

### 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	479/507 (94%)	460 (96%)	19 (4%)	27	35
1	B	474/507 (94%)	456 (96%)	18 (4%)	28	37
All	All	953/1014 (94%)	916 (96%)	37 (4%)	27	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	165	ILE
1	A	166	ASP
1	A	169	LYS
1	A	174	LYS
1	A	286	LEU
1	A	333	LEU
1	A	351	ASN
1	A	418	GLN
1	A	426	LEU
1	A	442	SER
1	A	461	THR
1	A	470	THR
1	A	471	SER
1	A	499	LEU
1	A	514	LYS
1	A	525	LYS
1	A	599	VAL
1	B	36	ASP
1	B	103	LYS
1	B	104	ASP
1	B	127	GLN
1	B	174	LYS
1	B	281	GLU
1	B	286	LEU
1	B	333	LEU
1	B	351	ASN
1	B	390	ASN
1	B	396	ASN
1	B	426	LEU
1	B	458	MET
1	B	461	THR
1	B	499	LEU
1	B	509	ASP
1	B	571	ASP
1	B	601	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	178	GLN
1	A	324	ASN
1	A	351	ASN
1	A	387	ASN
1	A	390	ASN
1	A	418	GLN
1	A	428	ASN
1	A	455	ASN
1	A	485	ASN
1	A	592	HIS
1	B	101	ASN
1	B	114	ASN
1	B	127	GLN
1	B	177	GLN
1	B	178	GLN
1	B	351	ASN
1	B	387	ASN
1	B	390	ASN
1	B	418	GLN
1	B	428	ASN
1	B	455	ASN
1	B	485	ASN
1	B	518	GLN
1	B	531	ASN
1	B	563	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 for Mogul analysis.

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	1611	-	4,4,4	0.33	0	6,6,6	0.49	0
4	ACT	B	1620	-	3,3,3	0.99	0	3,3,3	0.97	0
3	SO4	A	1615	-	4,4,4	0.67	0	6,6,6	1.14	1 (16%)
3	SO4	B	1615	-	4,4,4	0.45	0	6,6,6	0.26	0
3	SO4	A	1620	-	4,4,4	0.34	0	6,6,6	0.37	0
3	SO4	A	1619	-	4,4,4	0.34	0	6,6,6	0.48	0
3	SO4	A	1618	-	4,4,4	0.45	0	6,6,6	0.87	0
3	SO4	A	1617	-	4,4,4	0.47	0	6,6,6	0.87	0
3	SO4	B	1617	-	4,4,4	0.38	0	6,6,6	0.66	0
3	SO4	A	1613	-	4,4,4	0.18	0	6,6,6	0.34	0
3	SO4	A	1612	-	4,4,4	0.26	0	6,6,6	0.32	0
3	SO4	B	1616	-	4,4,4	0.43	0	6,6,6	0.33	0
3	SO4	A	1614	-	4,4,4	0.32	0	6,6,6	0.47	0
3	SO4	B	1614	-	4,4,4	0.23	0	6,6,6	0.31	0
3	SO4	B	1613	-	4,4,4	0.14	0	6,6,6	0.52	0
3	SO4	A	1621	1	4,4,4	0.99	0	6,6,6	1.66	1 (16%)
3	SO4	B	1619	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)
3	SO4	A	1616	1	4,4,4	0.48	0	6,6,6	0.57	0
3	SO4	B	1618	-	4,4,4	0.42	0	6,6,6	0.83	0
3	SO4	B	1612	-	4,4,4	0.48	0	6,6,6	0.87	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1621	SO4	O4-S-O3	3.83	125.39	109.06
3	B	1619	SO4	O4-S-O3	3.82	125.36	109.06
3	A	1615	SO4	O4-S-O3	2.10	118.05	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1619	SO4	1	0
3	B	1616	SO4	1	0
3	B	1613	SO4	1	0
3	A	1621	SO4	1	0
3	B	1619	SO4	2	0
3	A	1616	SO4	4	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	571/608 (93%)	1.07	77 (13%) <b>8</b> <b>6</b>	2, 26, 45, 79	4 (0%)
1	B	566/608 (93%)	1.13	64 (11%) <b>11</b> <b>9</b>	2, 19, 33, 57	2 (0%)
All	All	1137/1216 (93%)	1.10	141 (12%) <b>9</b> <b>7</b>	2, 22, 41, 79	6 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	ILE	8.7
1	A	502	ALA	6.4
1	A	508	ILE	6.3
1	A	603	GLY	5.8
1	A	231	ARG	5.7
1	B	502	ALA	4.6
1	A	504	SER	4.3
1	A	432	ARG	4.3
1	A	606	VAL	4.2
1	B	432	ARG	4.1
1	A	602	ASP	4.1
1	A	549	ALA	4.1
1	B	148	ALA	4.1
1	B	510	TYR	4.0
1	A	187	CYS	4.0
1	B	441	GLY	3.9
1	A	104	ASP	3.5
1	A	505	ASN	3.5
1	A	501	TYR	3.5
1	A	157	VAL	3.5
1	A	604	LYS	3.5
1	A	141	VAL	3.4
1	A	507	ASN	3.4
1	B	594	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	501	TYR	3.2
1	B	103	LYS	3.2
1	B	545	THR	3.2
1	A	166	ASP	3.2
1	A	503	ASP	3.2
1	B	603	GLY	3.2
1	A	169	LYS	3.2
1	B	417	GLU	3.2
1	A	546	ALA	3.1
1	B	512	PRO	3.0
1	B	416	GLN	3.0
1	B	602	ASP	3.0
1	A	593	PHE	3.0
1	A	506	ALA	3.0
1	A	510	TYR	2.9
1	A	509	ASP	2.9
1	A	605	PRO	2.9
1	A	152	ALA	2.9
1	A	256	GLY	2.9
1	B	65	LYS	2.9
1	A	118	ILE	2.8
1	B	509	ASP	2.8
1	A	162	PHE	2.8
1	B	575	SER	2.8
1	A	163	GLY	2.8
1	A	442	SER	2.8
1	B	413	GLU	2.8
1	B	599	VAL	2.8
1	A	103	LYS	2.7
1	B	515	ILE	2.7
1	A	251	ASN	2.7
1	A	135	ALA	2.7
1	B	522	PHE	2.7
1	A	171	LEU	2.7
1	A	513	ALA	2.7
1	A	515	ILE	2.7
1	A	511	PRO	2.6
1	A	159	VAL	2.6
1	A	164	ALA	2.6
1	A	79	GLY	2.6
1	A	514	LYS	2.6
1	B	592	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	577	PHE	2.6
1	A	512	PRO	2.6
1	B	139	LEU	2.6
1	B	587	GLY	2.6
1	A	315	ALA	2.5
1	B	152	ALA	2.5
1	B	513	ALA	2.5
1	B	511	PRO	2.5
1	B	544	ASP	2.5
1	A	76	LYS	2.5
1	A	77	LEU	2.5
1	B	447	TRP	2.5
1	B	251	ASN	2.5
1	B	423	GLY	2.5
1	B	499	LEU	2.5
1	B	591	TRP	2.5
1	A	74	ALA	2.5
1	A	234	PRO	2.4
1	B	535	LYS	2.4
1	A	165	ILE	2.4
1	A	137	GLY	2.4
1	A	156	ILE	2.4
1	A	418	GLN	2.4
1	B	604	LYS	2.4
1	A	130	VAL	2.4
1	A	601	VAL	2.4
1	B	57	TRP	2.4
1	A	499	LEU	2.3
1	A	596	VAL	2.3
1	A	550	TRP	2.3
1	A	139	LEU	2.3
1	A	411	THR	2.3
1	B	130	VAL	2.3
1	B	601	VAL	2.3
1	B	151	SER	2.3
1	A	117	VAL	2.3
1	B	137	GLY	2.3
1	A	575	SER	2.3
1	B	357	ILE	2.2
1	B	411	THR	2.2
1	B	470	THR	2.2
1	B	442	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	GLY	2.2
1	B	323	LYS	2.2
1	B	597	LYS	2.2
1	B	430	TYR	2.2
1	A	138	SER	2.2
1	B	37	ALA	2.2
1	B	175	ALA	2.2
1	B	104	ASP	2.2
1	A	229	GLY	2.2
1	A	599	VAL	2.2
1	A	589	THR	2.2
1	A	142	ALA	2.2
1	B	420	PRO	2.2
1	A	183	CYS	2.2
1	B	606	VAL	2.2
1	B	553	LEU	2.1
1	B	253	SER	2.1
1	B	281	GLU	2.1
1	A	174	LYS	2.1
1	A	471	SER	2.1
1	A	594	SER	2.1
1	B	451	ILE	2.1
1	B	549	ALA	2.1
1	B	471	SER	2.1
1	B	593	PHE	2.1
1	A	39	GLN	2.1
1	A	101	ASN	2.0
1	B	183	CYS	2.0
1	A	500	ASP	2.0
1	A	78	LEU	2.0
1	B	408	ALA	2.0
1	A	189	VAL	2.0
1	B	500	ASP	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NI	B	1611	1/1	0.29	0.31	136,136,136,136	0
3	SO4	A	1612	5/5	0.63	0.16	74,75,76,77	0
3	SO4	B	1615	5/5	0.72	0.32	49,53,53,56	0
3	SO4	B	1616	5/5	0.73	0.33	55,57,60,60	0
3	SO4	A	1616	5/5	0.74	0.33	50,51,53,54	0
3	SO4	B	1618	5/5	0.74	0.21	43,49,51,53	0
3	SO4	A	1611	5/5	0.75	0.23	50,50,55,55	0
3	SO4	A	1615	5/5	0.76	0.32	45,45,49,52	0
3	SO4	B	1613	5/5	0.79	0.19	58,60,60,62	0
4	ACT	B	1620	4/4	0.79	0.24	20,20,20,20	0
3	SO4	B	1614	5/5	0.80	0.19	51,52,54,55	0
3	SO4	A	1617	5/5	0.80	0.29	47,48,49,49	0
3	SO4	A	1618	5/5	0.80	0.32	52,55,57,57	0
3	SO4	B	1617	5/5	0.80	0.17	51,53,54,56	0
3	SO4	A	1620	5/5	0.80	0.32	43,46,50,50	0
3	SO4	B	1619	5/5	0.80	0.29	20,20,20,20	0
3	SO4	A	1613	5/5	0.80	0.21	62,63,64,64	0
3	SO4	B	1612	5/5	0.82	0.20	33,46,46,46	0
3	SO4	A	1619	5/5	0.82	0.24	46,47,47,49	0
3	SO4	A	1621	5/5	0.82	0.29	20,20,20,20	0
2	NI	A	1609	1/1	0.85	0.18	92,92,92,92	0
2	NI	A	1610	1/1	0.86	0.26	93,93,93,93	0
2	NI	A	1608	1/1	0.88	0.23	41,41,41,41	0
3	SO4	A	1614	5/5	0.88	0.13	38,38,41,41	0
2	NI	B	1608	1/1	0.92	0.14	29,29,29,29	0
2	NI	A	1607	1/1	0.93	0.13	33,33,33,33	0
2	NI	B	1610	1/1	0.94	0.08	35,35,35,35	0
2	NI	B	1609	1/1	0.94	0.24	38,38,38,38	0
2	NI	B	1607	1/1	0.98	0.13	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.