



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WVU
Title : CRYSTAL STRUCTURE OF A MICHAELIS COMPLEX OF ALPHA-L-FUCOSIDASE GH29 FROM BACTEROIDES THETA IOTAOMICRON WITH THE SYNTHETIC SUBSTRATE 4-NITROPHENYL-ALPHA-L-FUCOSE
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Deposited on : 2009-10-20
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

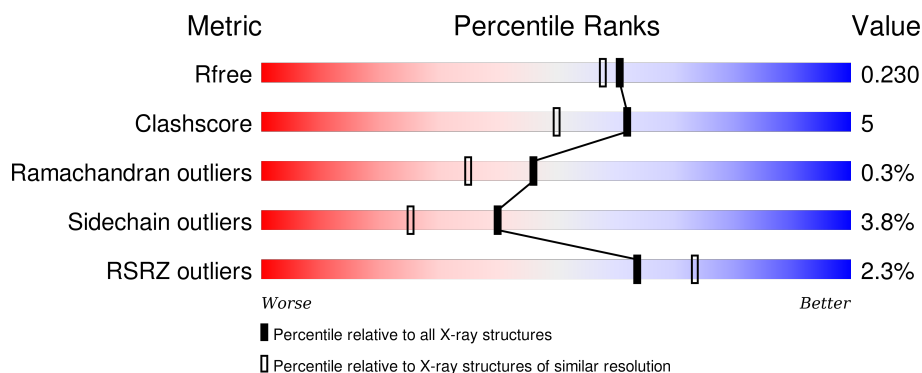
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	443	<div> <div>5%</div> <div>87%</div> <div>10% ..</div> </div>
1	B	443	<div> <div>87%</div> <div>9% ..</div> </div>
1	C	443	<div> <div>2%</div> <div>86%</div> <div>11% ..</div> </div>
1	D	443	<div> <div>2%</div> <div>86%</div> <div>10% ..</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	SO4	C	1473	-	-	-	X
2	SO4	D	1473	-	-	X	X
3	147	A	2001	X	-	-	-
3	147	B	2001	X	-	-	-
3	147	C	2001	X	-	-	-
3	147	D	2001	X	-	-	-

2 Entry composition [i](#)

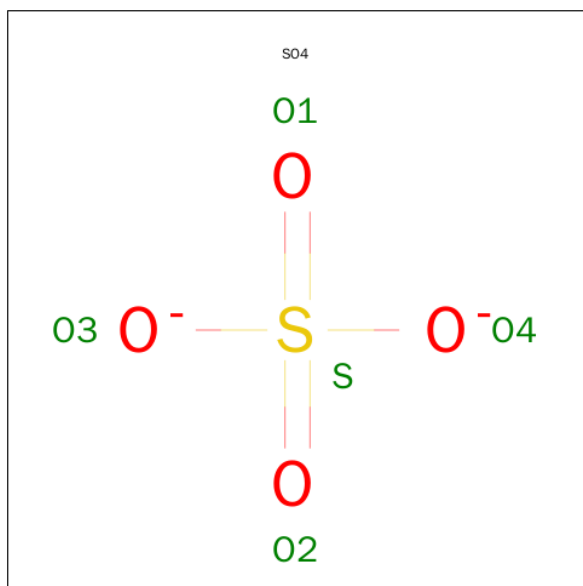
There are 4 unique types of molecules in this entry. The entry contains 15760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-L-FUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			
1	B	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			
1	C	437	Total	C	N	O	S	0	1	0
			3565	2292	601	655	17			
1	D	437	Total	C	N	O	S	0	0	0
			3562	2290	601	655	16			

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



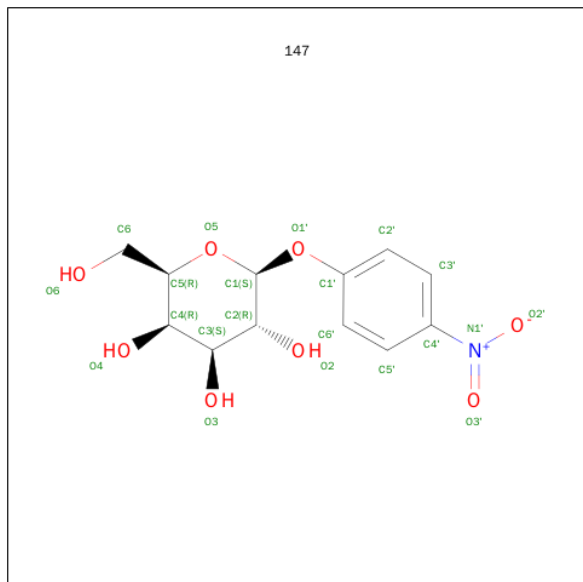
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is SUGAR (1-O-[P-NITROPHENYL]-BETA-D-GALACTOPYRANOSE) (three-letter code: 147) (formula: C₁₂H₁₅NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	12	1	7		
3	B	1	Total	C	N	O	0	0
			20	12	1	7		
3	C	1	Total	C	N	O	0	0
			20	12	1	7		
3	D	1	Total	C	N	O	0	0
			20	12	1	7		

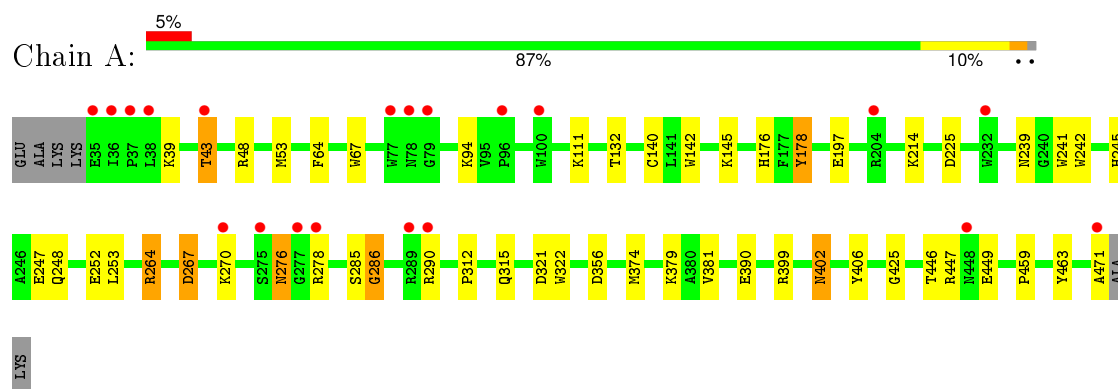
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	306	Total 306	O 306	0	0
4	B	342	Total 342	O 342	0	0
4	C	390	Total 390	O 390	0	0
4	D	356	Total 356	O 356	0	0

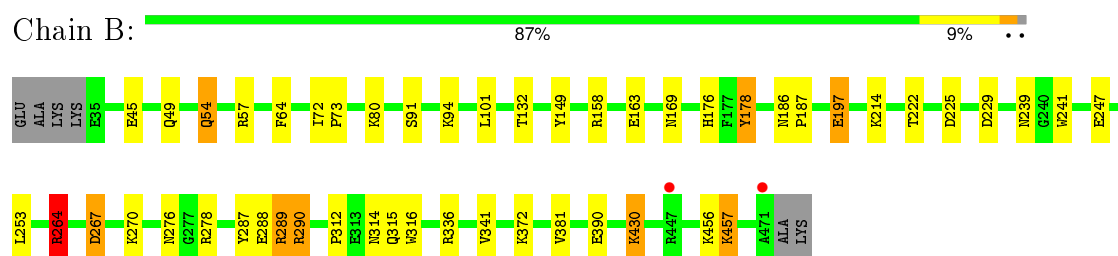
3 Residue-property plots [i](#)

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

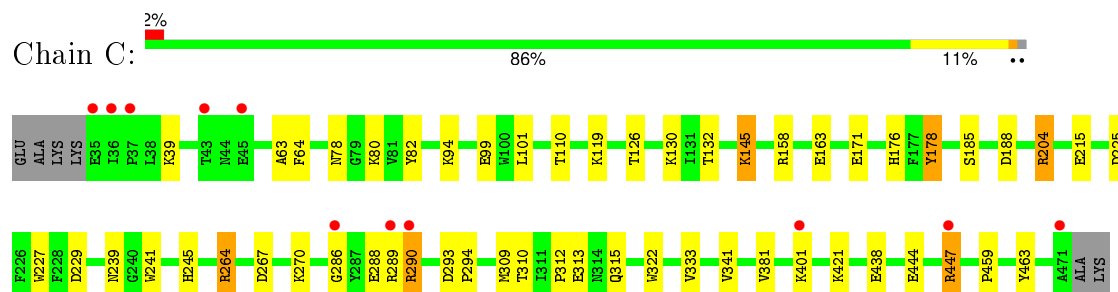
• Molecule 1: ALPHA-L-FUCOSIDASE



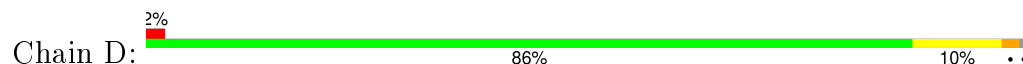
• Molecule 1: ALPHA-L-FUCOSIDASE

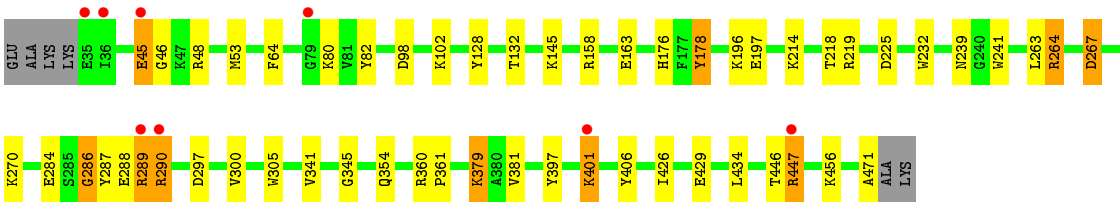


• Molecule 1: ALPHA-L-FUCOSIDASE



• Molecule 1: ALPHA-L-FUCOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.61Å 184.82Å 98.06Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	47.25 – 1.95 47.25 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.25-1.95) 98.3 (47.25-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.229 0.180 , 0.230	Depositor DCC
R_{free} test set	6950 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 138063 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15760	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 147, 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	0.61	0/3669	0.63	0/4976
1	B	0.68	0/3669	0.68	4/4976 (0.1%)
1	C	0.68	0/3675	0.74	4/4984 (0.1%)
1	D	0.67	0/3669	0.70	2/4976 (0.0%)
All	All	0.66	0/14682	0.69	10/19912 (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	D	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	C	204	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	C	264	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	D	264	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	D	264	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	B	264	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	B	264	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	264	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	289	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	289	ARG	NE-CZ-NH2	-5.73	117.44	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	263	LEU	Peptide
1	D	289	ARG	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	3562	0	3431	34	0
1	B	3562	0	3431	37	0
1	C	3565	0	3436	36	0
1	D	3562	0	3431	41	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	3	0
3	A	20	0	10	0	0
3	B	20	0	10	2	0
3	C	20	0	10	1	0
3	D	20	0	11	1	0
4	A	306	0	0	8	0
4	B	342	0	0	7	0
4	C	390	0	0	6	0
4	D	356	0	0	15	0
All	All	15760	0	13770	151	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 5.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:GLU:CD	4:D:2203:HOH:O	1.70	1.24
1:D:289:ARG:HG3	1:D:290:ARG:HB2	1.37	1.04
1:C:145:LYS:HD2	4:D:2182:HOH:O	1.55	1.03
1:C:145:LYS:CD	4:D:2182:HOH:O	2.05	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASN:HD22	1:A:241:TRP:HE1	1.15	0.95
1:C:188:ASP:OD2	1:C:204:ARG:HD2	1.68	0.92
1:B:239:ASN:HD22	1:B:241:TRP:HE1	1.19	0.91
1:A:379:LYS:HE2	1:A:406:TYR:OH	1.77	0.85
1:D:239:ASN:HD22	1:D:241:TRP:HE1	1.25	0.84
1:A:390:GLU:OE2	4:A:2234:HOH:O	1.94	0.84
2:D:1473:SO4:O4	4:D:2356:HOH:O	1.97	0.83
1:C:239:ASN:HD22	1:C:241:TRP:HE1	1.26	0.82
1:C:438:GLU:OE2	4:C:2357:HOH:O	2.00	0.79
1:C:421:LYS:CB	4:C:2369:HOH:O	2.29	0.79
1:D:286:GLY:O	1:D:290:ARG:NH1	2.16	0.78
1:C:289:ARG:HD3	1:C:310:THR:OG1	1.84	0.77
2:D:1473:SO4:S	4:D:2356:HOH:O	2.43	0.77
1:D:284:GLU:OE1	1:D:287:TYR:CE1	2.38	0.76
1:D:289:ARG:CG	1:D:290:ARG:HB2	2.17	0.74
1:D:45:GLU:HG2	1:D:46:GLY:N	2.03	0.73
1:A:402:ASN:ND2	4:A:2246:HOH:O	2.23	0.70
1:A:312:PRO:HG2	1:A:315:GLN:HB2	1.73	0.70
1:D:98:ASP:O	1:D:102:LYS:HG3	1.91	0.70
1:D:284:GLU:OE2	4:D:2203:HOH:O	1.93	0.70
1:A:239:ASN:ND2	1:A:241:TRP:HE1	1.87	0.70
2:D:1473:SO4:O2	4:D:2356:HOH:O	2.10	0.70
1:D:401:LYS:HG3	4:D:2025:HOH:O	1.90	0.69
1:A:399:ARG:HD3	4:A:2244:HOH:O	1.92	0.69
1:C:312:PRO:HG2	1:C:315:GLN:HB2	1.74	0.69
1:A:399:ARG:CD	4:A:2244:HOH:O	2.41	0.68
1:B:336:ARG:NH1	4:B:2250:HOH:O	2.26	0.68
1:B:276:ASN:HD22	1:B:278:ARG:HH22	1.40	0.67
1:D:284:GLU:OE1	1:D:287:TYR:HE1	1.77	0.66
1:B:430:LYS:HE2	4:B:2314:HOH:O	1.95	0.66
1:B:49:GLN:HE22	1:B:57:ARG:HH12	1.43	0.66
1:C:176:HIS:CG	1:C:225:ASP:HB3	2.30	0.66
1:A:446:THR:HG22	1:A:449:GLU:HB3	1.79	0.64
1:A:111:LYS:HE2	1:A:356:ASP:OD2	1.96	0.64
1:A:278:ARG:NH1	4:A:2160:HOH:O	2.31	0.64
1:D:289:ARG:HG3	1:D:290:ARG:CB	2.21	0.62
1:D:45:GLU:HG2	1:D:46:GLY:H	1.65	0.62
1:B:289:ARG:HH22	1:B:316:TRP:HE1	1.47	0.61
1:D:176:HIS:CG	1:D:225:ASP:HB3	2.35	0.61
1:D:45:GLU:CG	1:D:46:GLY:H	2.12	0.60
1:A:176:HIS:CG	1:A:225:ASP:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLU:O	1:C:290:ARG:HG2	2.02	0.59
1:B:456:LYS:HB3	1:B:457:LYS:HE2	1.84	0.59
1:B:132:THR:HA	1:B:178:TYR:HB3	1.86	0.57
1:D:45:GLU:CG	1:D:46:GLY:N	2.67	0.57
1:B:312:PRO:HG2	1:B:315:GLN:HB2	1.87	0.57
1:B:176:HIS:CG	1:B:225:ASP:HB3	2.41	0.56
1:C:158:ARG:HD2	1:C:163:GLU:OE2	2.06	0.56
1:A:267:ASP:N	1:A:267:ASP:OD2	2.39	0.55
1:D:289:ARG:CA	1:D:290:ARG:HB2	2.36	0.55
1:A:425:GLY:O	1:A:471:ALA:C	2.45	0.54
1:D:426:ILE:HD13	1:D:471:ALA:HA	1.88	0.54
1:B:197:GLU:O	1:B:197:GLU:OE1	2.25	0.54
1:D:48:ARG:HB2	1:D:53:MET:HG2	1.88	0.54
1:B:276:ASN:HD22	1:B:278:ARG:NH2	2.06	0.53
1:C:130:LYS:HE2	1:C:227:TRP:CD1	2.45	0.52
1:A:48:ARG:HB2	1:A:53:MET:HG2	1.92	0.52
1:C:239:ASN:ND2	1:C:241:TRP:HE1	2.04	0.52
1:A:276:ASN:N	1:A:276:ASN:HD22	2.08	0.51
1:A:399:ARG:HD2	4:A:2244:HOH:O	2.09	0.51
1:C:289:ARG:CD	4:C:2285:HOH:O	2.59	0.51
1:D:284:GLU:OE1	4:D:2203:HOH:O	2.06	0.50
1:C:178:TYR:CD2	1:C:178:TYR:C	2.84	0.50
1:B:158:ARG:HD2	1:B:163:GLU:OE2	2.11	0.50
1:B:289:ARG:NH2	1:B:316:TRP:HE1	2.10	0.50
1:A:140:CYS:HB3	1:A:142:TRP:CE3	2.47	0.49
1:A:214:LYS:HG2	1:A:253:LEU:HD11	1.94	0.49
1:A:178:TYR:CD2	1:A:178:TYR:C	2.86	0.49
1:D:397:TYR:HA	1:D:406:TYR:O	2.12	0.49
1:D:158:ARG:HD2	1:D:163:GLU:OE2	2.12	0.49
1:C:459:PRO:HG2	1:C:463:TYR:CG	2.47	0.49
1:A:312:PRO:HG3	1:A:322:TRP:CE2	2.48	0.49
1:B:372:LYS:NZ	4:B:2269:HOH:O	2.46	0.48
1:A:459:PRO:HG2	1:A:463:TYR:CG	2.48	0.48
1:A:374:MET:HE1	1:A:381:VAL:HG11	1.95	0.48
1:D:354:GLN:NE2	4:D:2254:HOH:O	2.47	0.48
1:D:132:THR:HA	1:D:178:TYR:HB3	1.95	0.48
1:A:140:CYS:HB3	1:A:142:TRP:CZ3	2.49	0.48
1:B:49:GLN:NE2	1:B:57:ARG:HH12	2.11	0.48
1:D:305:TRP:CE2	1:D:345:GLY:HA3	2.49	0.48
1:C:119:LYS:HE3	1:C:171:GLU:OE2	2.13	0.48
1:A:248:GLN:HE21	1:A:252:GLU:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:TYR:HB3	4:D:2204:HOH:O	2.13	0.47
1:D:214:LYS:O	1:D:218:THR:HG23	2.13	0.47
1:D:239:ASN:ND2	1:D:241:TRP:HE1	2.04	0.47
1:A:132:THR:HA	1:A:178:TYR:HB3	1.96	0.47
1:C:94:LYS:HD3	4:C:2067:HOH:O	2.13	0.47
1:D:80:LYS:HD3	1:D:82:TYR:CZ	2.50	0.46
1:D:128:TYR:CD1	1:D:176:HIS:CE1	3.03	0.46
1:D:178:TYR:CD2	1:D:178:TYR:C	2.89	0.46
1:C:101:LEU:HD11	1:C:185:SER:HB2	1.98	0.46
1:A:276:ASN:H	1:A:276:ASN:HD22	1.63	0.46
1:C:459:PRO:HG2	1:C:463:TYR:CD1	2.51	0.46
1:C:188:ASP:OD2	1:C:204:ARG:CD	2.52	0.46
1:B:289:ARG:NH2	1:B:314:ASN:OD1	2.48	0.46
1:A:43:THR:OG1	4:A:2003:HOH:O	2.21	0.46
1:C:312:PRO:HG3	1:C:322:TRP:CE2	2.51	0.45
1:C:145:LYS:CE	4:D:2182:HOH:O	2.55	0.45
1:C:119:LYS:HB3	4:C:2108:HOH:O	2.17	0.45
1:C:80:LYS:HD3	1:C:82:TYR:CZ	2.52	0.45
1:A:276:ASN:ND2	1:A:276:ASN:N	2.65	0.45
1:B:390:GLU:OE2	4:B:2290:HOH:O	2.20	0.45
1:A:285:SER:HA	1:A:286:GLY:HA3	1.81	0.45
1:B:54:GLN:NE2	4:B:2025:HOH:O	2.46	0.44
1:B:278:ARG:HD3	4:B:2205:HOH:O	2.18	0.44
1:D:360:ARG:HB2	1:D:361:PRO:HD2	1.98	0.44
1:C:309:MET:HE1	1:C:333:VAL:HG22	1.99	0.44
1:B:267:ASP:OD2	1:B:267:ASP:N	2.50	0.44
1:B:72:ILE:HB	1:B:73:PRO:CD	2.48	0.44
1:B:80:LYS:HE3	4:B:2049:HOH:O	2.17	0.44
1:D:297:ASP:O	1:D:300:VAL:HG22	2.18	0.44
1:B:214:LYS:HG2	1:B:253:LEU:HD11	2.00	0.44
1:C:63:ALA:HB2	1:C:126:THR:HG21	1.99	0.43
1:C:447:ARG:HD2	1:C:447:ARG:HA	1.54	0.43
1:B:49:GLN:HE22	1:B:57:ARG:NH1	2.11	0.43
1:D:287:TYR:HD2	1:D:290:ARG:O	2.01	0.43
1:B:247:GLU:OE1	1:B:264:ARG:HD3	2.19	0.43
1:C:289:ARG:HD2	1:C:313:GLU:O	2.18	0.43
1:D:401:LYS:CG	4:D:2025:HOH:O	2.59	0.43
1:B:430:LYS:HB2	1:B:430:LYS:HE3	1.63	0.42
1:C:145:LYS:HE3	4:D:2182:HOH:O	2.17	0.42
1:C:94:LYS:CD	4:C:2067:HOH:O	2.67	0.42
1:A:321:ASP:OD1	4:A:2187:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:CD2	1:B:178:TYR:C	2.92	0.42
1:A:247:GLU:OE1	1:A:264:ARG:HD3	2.20	0.42
1:C:293:ASP:HA	1:C:294:PRO:HD3	1.87	0.42
1:C:229:ASP:OD2	3:C:2001:147:H2	2.20	0.41
1:C:132:THR:HA	1:C:178:TYR:HB3	2.02	0.41
1:B:288:GLU:HB2	3:B:2001:147:O2'	2.21	0.41
1:C:145:LYS:HB2	1:C:215:GLU:OE1	2.20	0.41
1:D:446:THR:OG1	1:D:447:ARG:N	2.53	0.41
1:B:101:LEU:HD13	1:B:149:TYR:CE1	2.55	0.41
1:B:186:ASN:HA	1:B:187:PRO:HD2	1.88	0.41
1:B:197:GLU:OE1	1:B:197:GLU:C	2.59	0.41
1:B:229:ASP:OD2	3:B:2001:147:H2	2.20	0.41
1:B:91:SER:O	1:B:94:LYS:HD2	2.20	0.41
1:D:288:GLU:HB2	3:D:2001:147:O3'	2.21	0.41
1:B:341:VAL:HG21	1:B:381:VAL:HG13	2.03	0.41
1:C:341:VAL:HG21	1:C:381:VAL:HG13	2.02	0.41
1:D:429:GLU:HG2	4:D:2312:HOH:O	2.21	0.41
1:D:341:VAL:HG21	1:D:381:VAL:HG13	2.03	0.40
1:B:169:ASN:ND2	1:B:222:THR:OG1	2.49	0.40
1:B:287:TYR:H	1:B:290:ARG:HH21	1.68	0.40
1:A:241:TRP:CG	1:A:242:TRP:N	2.89	0.40
1:D:267:ASP:OD2	1:D:267:ASP:N	2.53	0.40
1:A:379:LYS:CE	1:A:406:TYR:OH	2.58	0.40
1:D:379:LYS:HD3	1:D:434:LEU:HD11	2.03	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	435/443 (98%)	416 (96%)	18 (4%)	1 (0%)	52 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/443 (98%)	424 (98%)	11 (2%)	0	100	100
1	C	436/443 (98%)	423 (97%)	12 (3%)	1 (0%)	52	43
1	D	435/443 (98%)	422 (97%)	10 (2%)	3 (1%)	26	14
All	All	1741/1772 (98%)	1685 (97%)	51 (3%)	5 (0%)	46	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	GLU
1	D	290	ARG
1	A	286	GLY
1	C	286	GLY
1	D	286	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	370/377 (98%)	354 (96%)	16 (4%)	35	20
1	B	370/377 (98%)	359 (97%)	11 (3%)	48	36
1	C	371/377 (98%)	356 (96%)	15 (4%)	38	23
1	D	370/377 (98%)	356 (96%)	14 (4%)	40	25
All	All	1481/1508 (98%)	1425 (96%)	56 (4%)	40	25

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	43	THR
1	A	64	PHE
1	A	67	TRP
1	A	94	LYS
1	A	145	LYS

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Mol	Chain	Res	Type
1	A	178	TYR
1	A	197	GLU
1	A	245	HIS
1	A	264	ARG
1	A	267	ASP
1	A	270	LYS
1	A	276	ASN
1	A	290	ARG
1	A	402	ASN
1	A	447	ARG
1	B	45	GLU
1	B	54	GLN
1	B	64	PHE
1	B	178	TYR
1	B	197	GLU
1	B	264	ARG
1	B	267	ASP
1	B	270	LYS
1	B	290	ARG
1	B	430	LYS
1	B	457	LYS
1	C	39	LYS
1	C	64	PHE
1	C	78	ASN
1	C	99	GLU
1	C	110	THR
1	C	145	LYS
1	C	178	TYR
1	C	245	HIS
1	C	264	ARG
1	C	267	ASP
1	C	270	LYS
1	C	290	ARG
1	C	401	LYS
1	C	444	GLU
1	C	447	ARG
1	D	64	PHE
1	D	145	LYS
1	D	178	TYR
1	D	196	LYS
1	D	197	GLU
1	D	219	ARG

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Mol	Chain	Res	Type
1	D	232	TRP
1	D	264	ARG
1	D	267	ASP
1	D	270	LYS
1	D	379	LYS
1	D	401	LYS
1	D	447	ARG
1	D	456	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	78	ASN
1	A	239	ASN
1	A	248	GLN
1	B	49	GLN
1	B	78	ASN
1	B	239	ASN
1	C	49	GLN
1	C	54	GLN
1	C	78	ASN
1	C	239	ASN
1	D	44	ASN
1	D	54	GLN
1	D	169	ASN
1	D	239	ASN
1	D	354	GLN

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

11 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	1472	-	4,4,4	0.32	0	6,6,6	0.28	0
3	147	A	2001	-	19,21,22	3.35	2 (10%)	28,30,31	1.76	6 (21%)
2	SO4	B	1472	-	4,4,4	0.52	0	6,6,6	0.16	0
3	147	B	2001	-	19,21,22	3.11	3 (15%)	28,30,31	1.84	6 (21%)
2	SO4	C	1472	-	4,4,4	0.55	0	6,6,6	0.29	0
2	SO4	C	1473	-	4,4,4	0.36	0	6,6,6	0.47	0
3	147	C	2001	-	19,21,22	3.45	4 (21%)	28,30,31	1.81	6 (21%)
2	SO4	D	1472	-	4,4,4	0.41	0	6,6,6	0.22	0
2	SO4	D	1473	-	4,4,4	0.40	0	6,6,6	0.12	0
2	SO4	D	1474	-	4,4,4	0.22	0	6,6,6	0.18	0
3	147	D	2001	-	19,21,22	3.37	4 (21%)	28,30,31	1.70	6 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1472	-	-	0/0/0/0	0/0/0/0
3	147	A	2001	-	4/4/6/6	0/8/28/30	0/2/2/2
2	SO4	B	1472	-	-	0/0/0/0	0/0/0/0
3	147	B	2001	-	4/4/6/6	0/8/28/30	0/2/2/2
2	SO4	C	1472	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1473	-	-	0/0/0/0	0/0/0/0
3	147	C	2001	-	4/4/6/6	0/8/28/30	0/2/2/2
2	SO4	D	1472	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1473	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1474	-	-	0/0/0/0	0/0/0/0
3	147	D	2001	-	4/4/6/6	0/8/28/30	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2001	147	O3-C3	-8.24	1.23	1.43
3	A	2001	147	O3-C3	-8.16	1.23	1.43
3	C	2001	147	O3-C3	-7.89	1.24	1.43
3	B	2001	147	O3-C3	-7.87	1.24	1.43
3	D	2001	147	O5-C1	2.00	1.47	1.41
3	B	2001	147	O1'-C1	2.74	1.45	1.41
3	C	2001	147	O5-C1	2.91	1.49	1.41
3	D	2001	147	O1'-C1	3.86	1.47	1.41
3	C	2001	147	O1'-C1	4.83	1.49	1.41
3	B	2001	147	O3'-N1'	10.01	1.42	1.22
3	D	2001	147	O3'-N1'	10.83	1.44	1.22
3	C	2001	147	O3'-N1'	10.93	1.44	1.22
3	A	2001	147	O3'-N1'	11.21	1.45	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	147	O4-C4-C3	-3.70	102.00	110.34
3	D	2001	147	O4-C4-C3	-3.38	102.72	110.34
3	C	2001	147	O4-C4-C3	-2.79	104.06	110.34
3	A	2001	147	O4-C4-C3	-2.26	105.25	110.34
3	C	2001	147	C3-C4-C5	2.00	113.10	109.72
3	D	2001	147	O1'-C1-C2	2.04	110.44	107.12
3	D	2001	147	O5-C1-O1'	2.07	113.92	108.39
3	A	2001	147	O1'-C1-C2	2.56	111.29	107.12
3	A	2001	147	O5-C5-C4	2.68	114.17	109.53
3	B	2001	147	O1'-C1-C2	2.69	111.50	107.12
3	B	2001	147	O5-C5-C4	2.98	114.69	109.53
3	B	2001	147	C4-C3-C2	3.05	116.49	110.79
3	C	2001	147	O1'-C1-C2	3.25	112.41	107.12
3	C	2001	147	C4-C3-C2	3.34	117.02	110.79
3	A	2001	147	O3-C3-C4	3.74	118.77	110.34
3	D	2001	147	C4-C3-C2	4.05	118.34	110.79
3	D	2001	147	O3-C3-C4	4.10	119.57	110.34
3	C	2001	147	O3-C3-C4	4.12	119.62	110.34
3	B	2001	147	O3-C3-C4	4.13	119.64	110.34
3	D	2001	147	O3-C3-C2	4.29	120.00	110.34
3	A	2001	147	C4-C3-C2	4.61	119.39	110.79
3	A	2001	147	O3-C3-C2	4.96	121.50	110.34
3	C	2001	147	O3-C3-C2	5.03	121.67	110.34
3	B	2001	147	O3-C3-C2	5.21	122.07	110.34

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2001	147	C2
3	A	2001	147	C3
3	A	2001	147	C4
3	A	2001	147	C5
3	C	2001	147	C2
3	C	2001	147	C3
3	C	2001	147	C4
3	C	2001	147	C5
3	D	2001	147	C2
3	D	2001	147	C3
3	D	2001	147	C4
3	D	2001	147	C5
3	B	2001	147	C2
3	B	2001	147	C3
3	B	2001	147	C4
3	B	2001	147	C5

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	147	2	0
3	C	2001	147	1	0
2	D	1473	SO4	3	0
3	D	2001	147	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	437/443 (98%)	0.27	20 (4%) 36 47	11, 23, 40, 50	1 (0%)
1	B	437/443 (98%)	-0.12	2 (0%) 91 95	9, 18, 30, 41	1 (0%)
1	C	437/443 (98%)	-0.10	11 (2%) 61 71	10, 16, 30, 48	1 (0%)
1	D	437/443 (98%)	-0.07	8 (1%) 71 80	10, 18, 30, 50	1 (0%)
All	All	1748/1772 (98%)	-0.01	41 (2%) 64 73	9, 18, 35, 50	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ARG	5.9
1	C	289	ARG	5.1
1	C	290	ARG	5.1
1	A	275	SER	4.2
1	A	471	ALA	3.6
1	A	79	GLY	3.6
1	D	36	ILE	3.5
1	D	447	ARG	3.5
1	A	37	PRO	3.4
1	D	289	ARG	3.2
1	A	277	GLY	3.2
1	C	471	ALA	3.1
1	A	204	ARG	3.0
1	D	45	GLU	3.0
1	A	38	LEU	3.0
1	C	36	ILE	3.0
1	C	45	GLU	2.9
1	A	278	ARG	2.9
1	A	290	ARG	2.8
1	A	36	ILE	2.8
1	A	270	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	43	THR	2.7
1	D	35	GLU	2.7
1	A	232	TRP	2.7
1	A	100	TRP	2.5
1	C	37	PRO	2.5
1	C	286	GLY	2.4
1	A	35	GLU	2.4
1	C	401	LYS	2.4
1	C	43	THR	2.4
1	B	471	ALA	2.3
1	D	290	ARG	2.3
1	C	35	GLU	2.3
1	A	77	TRP	2.2
1	D	79	GLY	2.2
1	A	448	ASN	2.2
1	A	78	ASN	2.1
1	D	401	LYS	2.1
1	B	447	ARG	2.1
1	C	447	ARG	2.1
1	A	96	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	1473	5/5	0.90	0.19	8.88	58,59,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	D	1473	5/5	0.93	0.43	7.10	96,96,96,97	0
3	147	B	2001	20/21	0.90	0.18	1.25	18,29,40,40	0
3	147	A	2001	20/21	0.83	0.26	0.99	28,37,47,47	0
3	147	D	2001	20/21	0.89	0.17	0.54	18,29,48,49	0
3	147	C	2001	20/21	0.86	0.17	0.24	16,25,40,41	0
2	SO4	D	1474	5/5	0.95	0.11	-0.69	73,73,73,73	0
2	SO4	D	1472	5/5	0.99	0.10	-0.88	31,32,33,33	0
2	SO4	A	1472	5/5	0.96	0.13	-	47,47,48,48	0
2	SO4	C	1472	5/5	0.98	0.12	-	40,41,41,42	0
2	SO4	B	1472	5/5	0.98	0.10	-	36,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.