Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:37 AM EDT

PDB ID	:	2WVS
Title	:	Crystal structure of an alpha-L-fucosidase GH29 trapped covalent intermediate from Bacteroides thetaiotaomicron in complex with 2- fluoro-fucosyl fluoride using an E288Q mutant
Authors	:	Lammerts van Bueren, A.; Ardevol, A.; Fayers-Kerr, J.; Luo, B.; Zhang, Y.; Sollogoub, M.; Bleriot, Y.; Rovira, C.; Davies, G.J.
Deposited on	:	2009-10-20
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

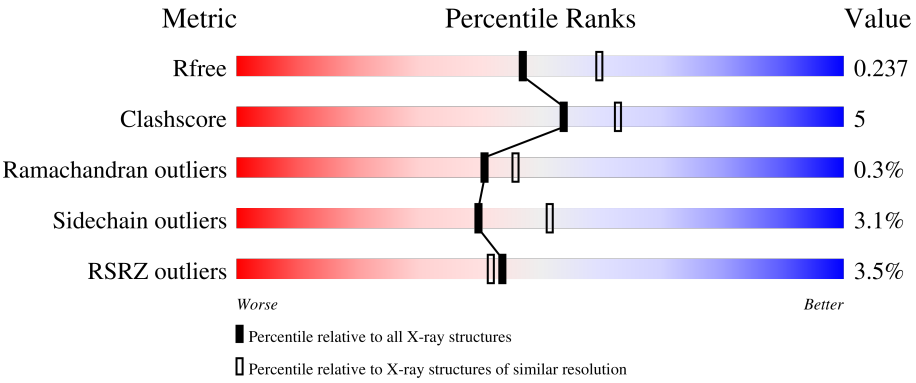
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 >=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 <=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	3% 86% 12%
1	B	443	2% 83% 14%
1	C	443	2% 84% 14%
1	D	443	7% 84% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15390 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.

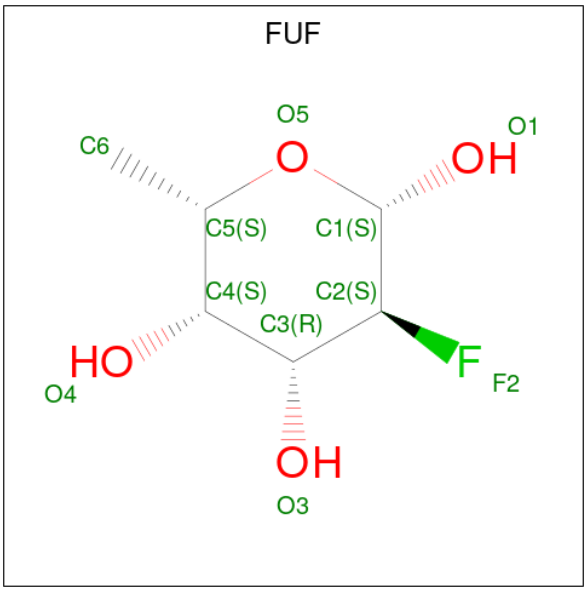
- Molecule 1 is a protein called ALPHA-L-FUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	2	0
			3598	2312	614	656	16			
1	B	437	Total	C	N	O	S	0	3	0
			3590	2308	612	654	16			
1	C	438	Total	C	N	O	S	0	4	0
			3605	2316	618	655	16			
1	D	438	Total	C	N	O	S	0	2	0
			3589	2306	612	655	16			

There are 4 discrepancies between the modelled and reference sequences:

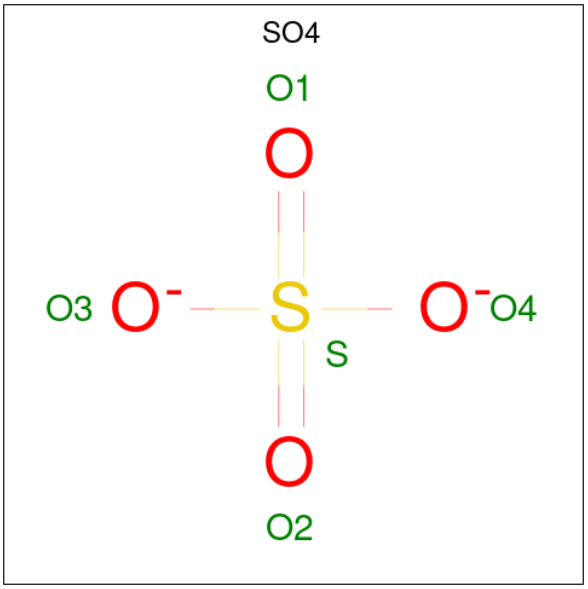
Chain	Residue	Modelled	Actual	Comment	Reference
A	288	GLN	GLU	engineered mutation	UNP Q8A3I4
B	288	GLN	GLU	engineered mutation	UNP Q8A3I4
C	288	GLN	GLU	engineered mutation	UNP Q8A3I4
D	288	GLN	GLU	engineered mutation	UNP Q8A3I4

- Molecule 2 is 2-deoxy-2-fluoro-beta-L-fucopyranose (three-letter code: FUF) (formula: $C_6H_{11}FO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F O 10 6 1 3	0	0
2	A	1	Total C F O 11 6 1 4	0	0
2	B	1	Total C F O 10 6 1 3	0	0
2	C	1	Total C F O 10 6 1 3	0	0
2	D	1	Total C F O 10 6 1 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

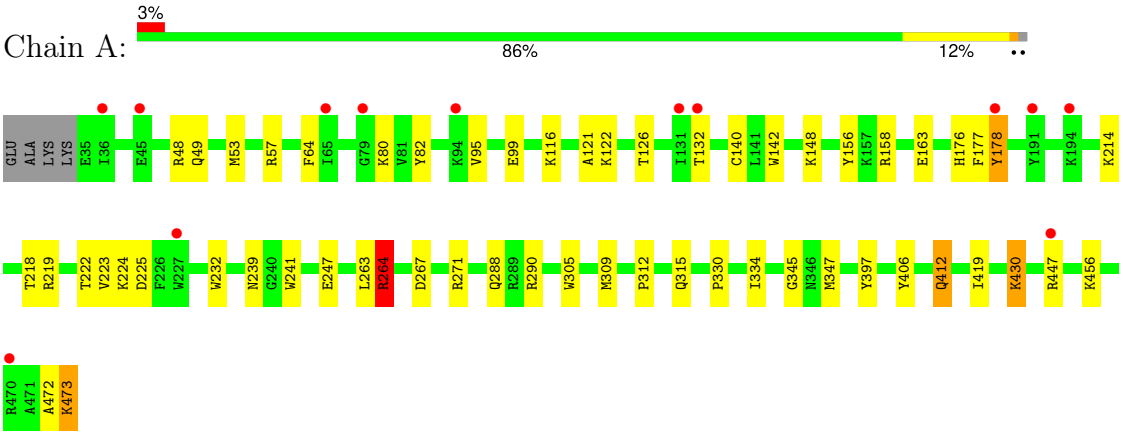
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	246	Total O 246 246	0	0
4	C	258	Total O 258 258	0	0
4	D	197	Total O 197 197	0	0

3 Residue-property plots (i)

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.

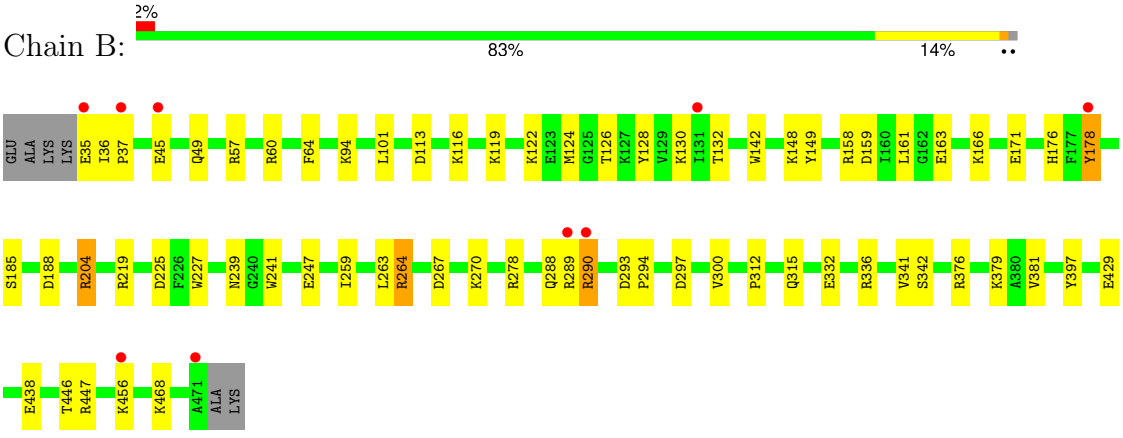
• Molecule 1: ALPHA-L-FUCOSIDASE

Chain A:



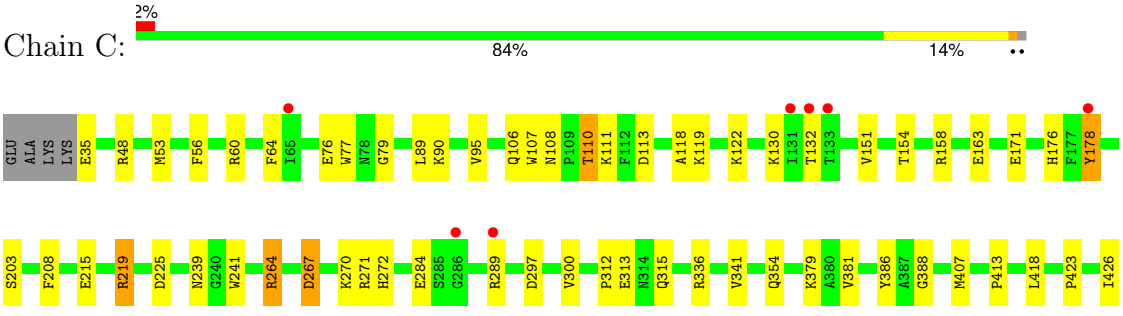
• Molecule 1: ALPHA-L-FUCOSIDASE

Chain B:



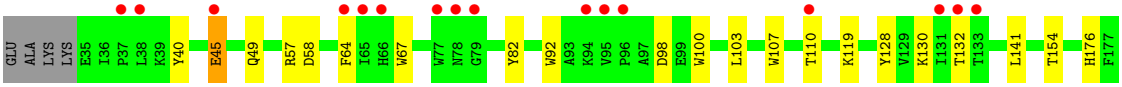
• Molecule 1: ALPHA-L-FUCOSIDASE

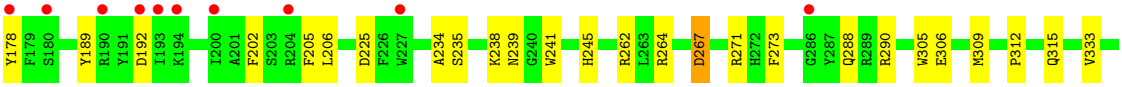
Chain C:

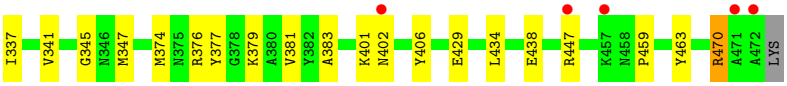


• Molecule 1: ALPHA-L-FUCOSIDASE

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.84Å 185.16Å 97.87Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	97.56 – 2.19 29.50 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.8 (97.56-2.19) 96.9 (29.50-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.178 , 0.235 0.180 , 0.237	Depositor DCC
R_{free} test set	4816 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15390	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, FUF

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	0.70	0/3711	0.72	1/5029 (0.0%)
1	B	0.71	0/3706	0.70	4/5022 (0.1%)
1	C	0.70	0/3724	0.72	2/5046 (0.0%)
1	D	0.68	0/3702	0.69	1/5018 (0.0%)
All	All	0.70	0/14843	0.71	8/20115 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	264	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	264	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	264	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	264	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	204	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	204	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	264	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	58	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	LEU	Peptide
1	B	263	LEU	Peptide

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	3598	0	3488	31	0
1	B	3590	0	3483	41	0
1	C	3605	0	3501	38	0
1	D	3589	0	3475	44	0
2	A	21	0	20	1	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	9	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	221	0	0	2	0
4	B	246	0	0	6	0
4	C	258	0	0	6	0
4	D	197	0	0	3	0
All	All	15390	0	13994	152	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 (152) 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:166:LYS:HE3	4:B:2075:HOH:O	1.17	1.27
1:D:192:ASP:HB2	4:D:2059:HOH:O	1.48	1.10
1:D:402:ASN:HB3	4:D:2161:HOH:O	1.59	1.02
1:B:239:ASN:HD22	1:B:241:TRP:HE1	1.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASN:HD22	1:C:241:TRP:HE1	1.19	0.88
1:D:239:ASN:HD22	1:D:241:TRP:HE1	1.24	0.85
1:D:429:GLU:OE2	1:D:470:ARG:HD2	1.82	0.79
1:A:49:GLN:HE22	1:A:57:ARG:HH12	1.34	0.75
1:B:166:LYS:CE	4:B:2075:HOH:O	1.94	0.75
1:D:130:LYS:HE3	1:D:306:GLU:OE1	1.88	0.73
1:B:290:ARG:HD3	4:B:2136:HOH:O	1.90	0.71
1:D:312:PRO:HG2	1:D:315:GLN:HB2	1.72	0.71
1:A:214:LYS:O	1:A:218:THR:HG23	1.93	0.69
1:B:188:ASP:OD2	1:B:204:ARG:HD2	1.92	0.69
1:B:60:ARG:HD2	1:B:341:VAL:HG22	1.77	0.67
1:A:176:HIS:CG	1:A:225:ASP:HB3	2.32	0.65
1:B:35:GLU:OE2	1:B:278:ARG:NH2	2.31	0.64
1:C:312:PRO:HG2	1:C:315:GLN:HB2	1.80	0.63
1:B:176:HIS:CG	1:B:225:ASP:HB3	2.32	0.63
1:C:176:HIS:CG	1:C:225:ASP:HB3	2.34	0.63
1:A:239:ASN:HD22	1:A:241:TRP:HE1	1.45	0.63
1:D:379:LYS:HD3	1:D:434:LEU:HD11	1.80	0.62
1:C:433:LEU:HD13	1:C:455:PRO:HG3	1.80	0.62
1:D:132:THR:O	1:D:141:LEU:HD12	2.00	0.61
1:D:239:ASN:ND2	1:D:241:TRP:HE1	1.95	0.61
1:A:239:ASN:ND2	1:A:241:TRP:HE1	1.99	0.60
1:D:379:LYS:HE2	1:D:406:TYR:OH	2.00	0.60
1:B:312:PRO:HG2	1:B:315:GLN:HB2	1.85	0.59
1:A:158:ARG:HD2	1:A:163:GLU:OE2	2.02	0.58
1:A:49:GLN:NE2	1:A:57:ARG:HH12	2.02	0.57
1:D:49:GLN:HE22	1:D:57:ARG:HH12	1.53	0.56
1:D:234:ALA:O	1:D:238:LYS:HG2	2.06	0.56
1:D:402:ASN:CB	4:D:2161:HOH:O	2.35	0.56
1:D:176:HIS:CG	1:D:225:ASP:HB3	2.42	0.55
1:C:130:LYS:HG2	1:C:176:HIS:HB2	1.88	0.55
1:C:354:GLN:NE2	4:C:2182:HOH:O	2.40	0.55
1:C:215:GLU:O	1:C:219:ARG:HB2	2.05	0.55
1:D:128:TYR:CD1	1:D:176:HIS:CE1	2.95	0.55
1:A:419:ILE:HG13	4:A:2188:HOH:O	2.06	0.55
1:C:289:ARG:HG2	4:C:2154:HOH:O	2.06	0.55
1:A:148:LYS:HE3	2:A:1450:FUF:H6C2	1.89	0.54
1:D:267:ASP:N	1:D:267:ASP:OD1	2.38	0.54
1:D:309:MET:CE	1:D:333:VAL:HG22	2.38	0.54
1:B:158:ARG:HD2	1:B:163:GLU:OE2	2.08	0.53
1:B:288:GLN:O	1:B:289:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HH22	1:B:166:LYS:NZ	2.05	0.53
1:A:397:TYR:HA	1:A:406:TYR:O	2.09	0.53
1:D:40:TYR:O	1:D:264:ARG:NH2	2.42	0.53
1:B:178:TYR:C	1:B:178:TYR:CD2	2.82	0.52
1:D:376:ARG:HG2	1:D:377:TYR:CE2	2.44	0.52
1:D:262:ARG:HH22	1:D:288:GLN:NE2	2.08	0.52
1:A:132:THR:HA	1:A:178:TYR:HB3	1.90	0.52
1:A:80:LYS:HD3	1:A:82:TYR:CZ	2.45	0.52
1:B:342:SER:HB2	1:B:397:TYR:O	2.10	0.51
1:A:222:THR:O	1:A:224:LYS:HE2	2.11	0.51
1:D:383:ALA:HB1	1:D:401:LYS:HD2	1.92	0.51
1:D:132:THR:HA	1:D:178:TYR:HB3	1.92	0.51
1:C:430:LYS:HD2	4:C:2237:HOH:O	2.11	0.51
1:C:271:ARG:O	1:C:272:HIS:HB2	2.11	0.51
1:D:49:GLN:NE2	1:D:57:ARG:HH12	2.09	0.51
1:A:95:VAL:CG1	1:A:99:GLU:HG2	2.40	0.50
1:C:433:LEU:HD13	1:C:455:PRO:CG	2.42	0.50
1:B:341:VAL:HG21	1:B:381:VAL:HG13	1.93	0.50
1:C:289:ARG:HD2	1:C:313:GLU:O	2.11	0.50
1:D:429:GLU:OE2	1:D:470:ARG:CD	2.57	0.50
1:A:330:PRO:O	1:A:334:ILE:HG13	2.12	0.50
1:D:178:TYR:CD2	1:D:178:TYR:C	2.85	0.50
1:C:48:ARG:HB2	1:C:53:MET:HG2	1.93	0.50
1:C:297:ASP:O	1:C:300:VAL:HG22	2.11	0.50
1:B:332:GLU:HB3	1:B:336[A]:ARG:HH12	1.76	0.49
1:C:132:THR:HA	1:C:178:TYR:HB3	1.93	0.49
1:D:459:PRO:HG2	1:D:463:TYR:CG	2.46	0.49
1:B:122:LYS:HD2	1:B:171:GLU:OE1	2.11	0.49
1:A:219:ARG:HH22	1:B:166:LYS:HZ1	1.59	0.49
1:B:132:THR:HA	1:B:178:TYR:HB3	1.95	0.49
1:D:130:LYS:HE3	1:D:306:GLU:CD	2.33	0.48
1:D:202:PHE:CE2	1:D:206:LEU:HD21	2.49	0.48
1:B:148:LYS:HG2	4:B:2060:HOH:O	2.12	0.48
1:D:305:TRP:CE2	1:D:345:GLY:HA3	2.49	0.48
1:C:178:TYR:C	1:C:178:TYR:CD2	2.87	0.48
1:D:189:TYR:HB2	1:D:205:PHE:CE1	2.49	0.48
1:C:336[A]:ARG:HH11	1:C:336[A]:ARG:HG3	1.78	0.47
1:A:271:ARG:HD3	4:A:2105:HOH:O	2.14	0.47
1:B:219:ARG:HD2	4:B:2104:HOH:O	2.14	0.47
1:D:309:MET:HE1	1:D:333:VAL:HG22	1.97	0.47
1:C:122:LYS:HD2	1:C:171:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:HE22	1:A:57:ARG:NH1	2.07	0.47
1:D:202:PHE:O	1:D:206:LEU:HG	2.15	0.47
1:A:156:TYR:CE2	1:A:158:ARG:HB2	2.49	0.47
1:C:108:ASN:O	1:C:110:THR:HG22	2.15	0.47
1:B:247:GLU:HG3	1:B:259:ILE:HG13	1.97	0.47
1:B:130:LYS:HE2	1:B:227:TRP:CD1	2.50	0.46
1:B:456:LYS:HG2	4:B:2232:HOH:O	2.15	0.46
1:A:309:MET:HG2	1:A:347:MET:SD	2.55	0.46
1:C:76:GLU:OE2	1:C:79:GLY:HA2	2.13	0.46
1:C:158:ARG:NH2	4:C:2066:HOH:O	2.47	0.46
1:C:118:ALA:HB1	1:C:171:GLU:HG3	1.98	0.46
1:B:101:LEU:HD11	1:B:185:SER:HB2	1.98	0.45
1:B:297:ASP:O	1:B:300:VAL:HG22	2.16	0.45
1:B:142:TRP:HB3	1:B:161:LEU:HD23	1.98	0.45
1:C:107:TRP:HB3	1:C:154:THR:HB	1.98	0.45
1:A:312:PRO:HG2	1:A:315:GLN:HB2	1.99	0.45
1:B:119:LYS:HE3	1:B:171:GLU:OE2	2.16	0.45
1:C:267:ASP:OD2	1:C:267:ASP:N	2.49	0.45
1:A:430:LYS:HE3	1:A:430:LYS:HB2	1.66	0.45
1:A:247:GLU:OE1	1:A:264:ARG:HD3	2.17	0.44
1:B:101:LEU:HD13	1:B:149:TYR:CE1	2.52	0.44
1:D:262:ARG:HH12	1:D:288:GLN:HE22	1.66	0.44
1:B:49:GLN:HE22	1:B:57:ARG:HH12	1.63	0.44
1:A:177:PHE:CD2	1:A:223:VAL:HG21	2.52	0.44
1:B:130:LYS:HG2	1:B:176:HIS:HB2	2.00	0.44
1:C:77:TRP:HB2	1:C:89:LEU:HD21	2.00	0.44
1:A:48:ARG:HB2	1:A:53:MET:HG2	2.00	0.43
1:B:159:ASP:O	1:B:163:GLU:HG3	2.18	0.43
1:D:107:TRP:HB3	1:D:154:THR:HB	1.99	0.43
1:C:341:VAL:HG21	1:C:381:VAL:HG13	2.00	0.43
1:A:121:ALA:HB1	1:A:126:THR:OG1	2.19	0.43
1:C:35:GLU:N	4:C:2001:HOH:O	2.51	0.43
1:B:113:ASP:OD2	1:B:116:LYS:HG3	2.19	0.43
1:C:379:LYS:HD3	1:C:434:LEU:HD11	2.01	0.43
1:D:447:ARG:HA	1:D:447:ARG:HD2	1.85	0.43
1:D:100:TRP:O	1:D:103:LEU:HG	2.18	0.43
1:D:309:MET:HE2	1:D:333:VAL:HG22	2.00	0.43
1:C:426:ILE:HD13	1:C:471:ALA:HA	2.01	0.42
1:B:128:TYR:CD1	1:B:176:HIS:CE1	3.07	0.42
1:D:337:ILE:HA	1:D:347:MET:HG2	2.02	0.42
1:C:407:MET:O	1:C:464:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:CG	1:B:116:LYS:HG3	2.40	0.42
1:A:305:TRP:CE2	1:A:345:GLY:HA3	2.55	0.41
1:C:90:LYS:NZ	1:C:95:VAL:O	2.48	0.41
1:B:429:GLU:OE1	1:B:468:LYS:NZ	2.50	0.41
1:A:412:GLN:HE21	1:A:412:GLN:HA	1.86	0.41
1:C:158:ARG:HD3	1:C:163:GLU:OE2	2.21	0.41
1:C:423:PRO:HD2	1:C:426:ILE:HB	2.01	0.41
1:B:124:MET:HG2	1:B:126:THR:HG23	2.02	0.41
1:C:56:PHE:CD2	1:C:56:PHE:C	2.93	0.41
1:C:386:TYR:CZ	1:C:388:GLY:HA2	2.56	0.41
1:A:140:CYS:HB3	1:A:142:TRP:CZ3	2.56	0.41
1:C:106:GLN:HG3	4:C:2038:HOH:O	2.20	0.41
1:C:413:PRO:HG3	1:C:418:LEU:HD23	2.03	0.41
1:D:374:MET:HE1	1:D:381:VAL:HB	2.03	0.41
1:B:446:THR:OG1	1:B:447:ARG:N	2.53	0.41
1:C:113:ASP:C	1:C:113:ASP:OD1	2.58	0.41
1:A:472:ALA:O	1:A:473:LYS:HB3	2.21	0.40
1:B:94:LYS:HE3	1:B:94:LYS:HB3	1.85	0.40
1:D:141:LEU:HD23	1:D:141:LEU:HA	1.88	0.40
1:B:293:ASP:HA	1:B:294:PRO:HD3	1.93	0.40
1:D:82:TYR:CD1	1:D:92:TRP:HB3	2.56	0.40
1:D:202:PHE:CZ	1:D:235:SER:HB2	2.57	0.40
1:B:36:ILE:HA	1:B:37:PRO:HD3	1.98	0.40
1:D:271:ARG:O	1:D:273:PHE:N	2.54	0.40
1:D:341:VAL:HG21	1:D:381:VAL:HG13	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	439/443 (99%)	421 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/443 (99%)	418 (95%)	20 (5%)	0	100	100
1	C	440/443 (99%)	423 (96%)	15 (3%)	2 (0%)	29	31
1	D	438/443 (99%)	416 (95%)	19 (4%)	3 (1%)	22	22
All	All	1755/1772 (99%)	1678 (96%)	72 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	290	ARG
1	D	110	THR
1	C	60	ARG
1	D	45	GLU
1	C	471	ALA

5.3.2 Protein sidechains (i)

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	374/377 (99%)	360 (96%)	14 (4%)	34	43
1	B	374/377 (99%)	363 (97%)	11 (3%)	42	54
1	C	375/377 (100%)	362 (96%)	13 (4%)	36	46
1	D	373/377 (99%)	364 (98%)	9 (2%)	49	62
All	All	1496/1508 (99%)	1449 (97%)	47 (3%)	40	51

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

Mol	Chain	Res	Type
1	A	64	PHE
1	A	116	LYS
1	A	122	LYS
1	A	178	TYR
1	A	232	TRP
1	A	264	ARG

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Mol	Chain	Res	Type
1	A	267	ASP
1	A	288	GLN
1	A	290	ARG
1	A	412	GLN
1	A	430	LYS
1	A	447	ARG
1	A	456	LYS
1	A	473	LYS
1	B	45	GLU
1	B	64	PHE
1	B	178	TYR
1	B	264	ARG
1	B	267	ASP
1	B	270[A]	LYS
1	B	270[B]	LYS
1	B	290	ARG
1	B	376	ARG
1	B	379	LYS
1	B	438	GLU
1	C	64	PHE
1	C	110	THR
1	C	111	LYS
1	C	119	LYS
1	C	151	VAL
1	C	178	TYR
1	C	203	SER
1	C	208	PHE
1	C	219	ARG
1	C	264	ARG
1	C	267	ASP
1	C	270	LYS
1	C	284	GLU
1	D	45	GLU
1	D	64	PHE
1	D	67	TRP
1	D	98	ASP
1	D	119	LYS
1	D	245	HIS
1	D	267	ASP
1	D	438	GLU
1	D	470	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	GLN
1	A	54	GLN
1	A	78	ASN
1	A	239	ASN
1	A	288	GLN
1	A	354	GLN
1	A	412	GLN
1	A	466	GLN
1	B	49	GLN
1	B	54	GLN
1	B	78	ASN
1	B	239	ASN
1	B	354	GLN
1	C	78	ASN
1	C	239	ASN
1	C	302	GLN
1	C	354	GLN
1	C	392	GLN
1	D	49	GLN
1	D	54	GLN
1	D	78	ASN
1	D	239	ASN
1	D	288	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	C	1473	-	4,4,4	0.23	0	6,6,6	0.10	0
2	FUF	A	1449	1	10,10,11	1.65	2 (20%)	11,14,16	1.88	4 (36%)
2	FUF	A	1450	-	11,11,11	0.74	0	15,16,16	2.48	7 (46%)
2	FUF	D	1449	1	10,10,11	1.31	2 (20%)	11,14,16	2.15	3 (27%)
3	SO4	B	1472	-	4,4,4	0.22	0	6,6,6	0.25	0
2	FUF	B	1449	1	10,10,11	1.73	3 (30%)	11,14,16	3.20	4 (36%)
3	SO4	A	1474	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	A	1475	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	D	1474	-	4,4,4	0.27	0	6,6,6	0.20	0
2	FUF	C	1449	1	10,10,11	1.62	1 (10%)	11,14,16	2.75	5 (45%)
3	SO4	D	1473	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	C	1474	-	4,4,4	0.25	0	6,6,6	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUF	A	1449	1	-	-	0/1/1/1
2	FUF	A	1450	-	-	-	0/1/1/1
2	FUF	D	1449	1	-	-	0/1/1/1
2	FUF	B	1449	1	-	-	0/1/1/1
2	FUF	C	1449	1	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1449	FUF	C1-C2	4.17	1.57	1.52
2	A	1449	FUF	C1-C2	2.80	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1449	FUF	O5-C5	2.68	1.48	1.43
2	B	1449	FUF	O5-C1	2.63	1.48	1.43
2	A	1449	FUF	O5-C1	2.51	1.47	1.43
2	B	1449	FUF	C1-C2	2.44	1.55	1.52
2	D	1449	FUF	C1-C2	2.38	1.55	1.52
2	D	1449	FUF	O5-C5	2.10	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1449	FUF	F2-C2-C1	9.01	115.36	108.26
2	C	1449	FUF	F2-C2-C1	6.72	113.55	108.26
2	D	1449	FUF	F2-C2-C1	5.79	112.82	108.26
2	A	1450	FUF	O5-C5-C6	-4.62	96.48	106.74
2	A	1450	FUF	C1-O5-C5	-4.34	107.61	114.37
2	A	1450	FUF	C6-C5-C4	4.33	121.01	113.08
2	A	1449	FUF	F2-C2-C1	3.81	111.26	108.26
2	A	1449	FUF	C1-O5-C5	3.54	121.31	112.97
2	C	1449	FUF	O5-C5-C6	3.28	114.53	107.40
2	A	1450	FUF	O1-C1-O5	-3.22	100.85	110.41
2	B	1449	FUF	O3-C3-C2	-2.92	104.33	109.55
2	B	1449	FUF	C1-O5-C5	2.86	119.71	112.97
2	A	1450	FUF	F2-C2-C1	2.67	110.80	107.81
2	B	1449	FUF	O5-C5-C6	2.64	113.13	107.40
2	D	1449	FUF	C1-O5-C5	2.63	119.17	112.97
2	C	1449	FUF	O5-C5-C4	2.53	114.10	109.55
2	C	1449	FUF	C3-C4-C5	-2.44	106.11	109.81
2	A	1450	FUF	F2-C2-C3	2.37	110.86	108.81
2	C	1449	FUF	C6-C5-C4	-2.33	108.82	113.08
2	A	1449	FUF	C2-C3-C4	2.30	112.37	109.59
2	D	1449	FUF	O5-C5-C4	2.29	113.67	109.55
2	A	1449	FUF	O5-C5-C4	2.03	113.21	109.55
2	A	1450	FUF	O4-C4-C3	-2.02	105.61	110.38

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	1450	FUF	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^{th} 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	439/443 (99%)	0.02	13 (2%)	50	48	18, 28, 45, 61	1 (0%)
1	B	437/443 (98%)	-0.08	9 (2%)	63	61	17, 26, 42, 57	1 (0%)
1	C	438/443 (98%)	-0.03	9 (2%)	63	61	17, 27, 40, 51	1 (0%)
1	D	438/443 (98%)	0.25	31 (7%)	16	14	20, 32, 54, 64	1 (0%)
All	All	1752/1772 (98%)	0.04	62 (3%)	44	42	17, 28, 46, 64	4 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	TYR	4.4
1	B	37	PRO	4.1
1	D	472	ALA	4.1
1	C	286	GLY	4.0
1	A	36	ILE	4.0
1	D	193	ILE	3.7
1	D	194	LYS	3.6
1	A	45	GLU	3.5
1	D	45	GLU	3.4
1	D	132	THR	3.2
1	D	447	ARG	3.2
1	D	65	ILE	3.2
1	C	289	ARG	3.1
1	B	131	ILE	3.1
1	D	131	ILE	3.1
1	C	132	THR	2.9
1	D	286	GLY	2.8
1	B	456	LYS	2.8
1	C	131	ILE	2.8
1	C	178	TYR	2.7
1	B	178	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	289	ARG	2.7
1	B	290	ARG	2.7
1	A	227	TRP	2.6
1	A	131	ILE	2.6
1	A	132	THR	2.6
1	D	200	ILE	2.6
1	D	471	ALA	2.6
1	A	79	GLY	2.5
1	C	65	ILE	2.5
1	B	35	GLU	2.4
1	D	180	SER	2.4
1	D	38	LEU	2.4
1	A	178	TYR	2.4
1	A	470	ARG	2.4
1	D	457	LYS	2.3
1	D	64	PHE	2.3
1	D	133	THR	2.3
1	D	37	PRO	2.3
1	D	192	ASP	2.3
1	D	402	ASN	2.3
1	D	95	VAL	2.2
1	D	96	PRO	2.2
1	D	110	THR	2.2
1	C	133	THR	2.2
1	B	45	GLU	2.2
1	C	447	ARG	2.2
1	D	190	ARG	2.2
1	A	194	LYS	2.2
1	C	471	ALA	2.2
1	D	204	ARG	2.2
1	D	78	ASN	2.1
1	B	471	ALA	2.1
1	A	65	ILE	2.1
1	D	66	HIS	2.1
1	A	94	LYS	2.1
1	D	227	TRP	2.1
1	A	191	TYR	2.0
1	D	77	TRP	2.0
1	D	94	LYS	2.0
1	A	447	ARG	2.0
1	D	79	GLY	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 (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, 95^{th} 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^2)	Q<0.9
2	FUF	C	1449	10/11	0.87	0.18	37,39,40,42	0
2	FUF	A	1450	11/11	0.89	0.22	23,27,29,30	11
3	SO4	A	1475	5/5	0.91	0.15	84,85,85,85	0
2	FUF	D	1449	10/11	0.94	0.16	36,37,38,38	0
2	FUF	A	1449	10/11	0.94	0.15	25,29,31,35	0
3	SO4	D	1474	5/5	0.94	0.12	61,64,65,65	0
2	FUF	B	1449	10/11	0.96	0.11	22,27,28,30	0
3	SO4	C	1474	5/5	0.96	0.13	78,78,78,79	0
3	SO4	D	1473	5/5	0.96	0.13	64,64,64,64	0
3	SO4	A	1474	5/5	0.96	0.10	65,65,65,66	0
3	SO4	C	1473	5/5	0.98	0.11	47,48,49,49	0
3	SO4	B	1472	5/5	0.98	0.10	56,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.