Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:57 AM GMT

PDB ID	:	2EXI
Title	:	Structure of the family43 beta-Xylosidase D15G mutant from geobacillus stearothermophilus
Authors	:	Brux, C.; Niefind, K.; Shallom-Shezifi, D.; Shoham, Y.; Schomburg, D.
Deposited on	:	2005-11-08
Resolution	:	2.15 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

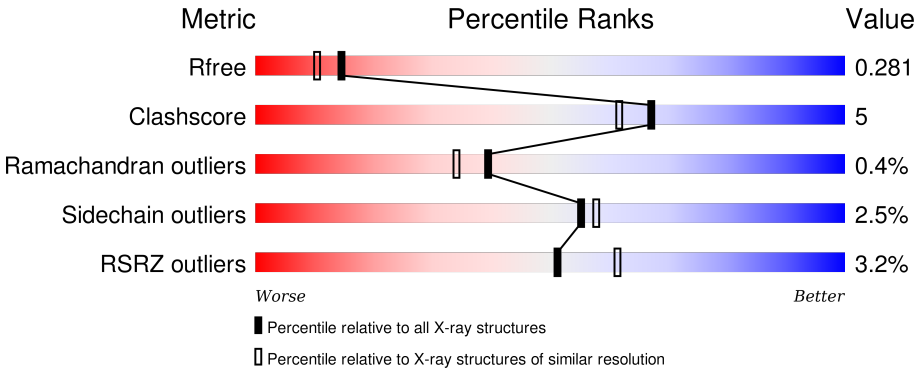
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 <=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	535	91% 8%
1	B	535	85% 14%
1	C	535	9% 84% 15%
1	D	535	89% 10%

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	MES	B	3006	-	-	-	X
3	MES	D	3007	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19639 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 beta-D-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			
1	B	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			
1	C	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			
1	D	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			

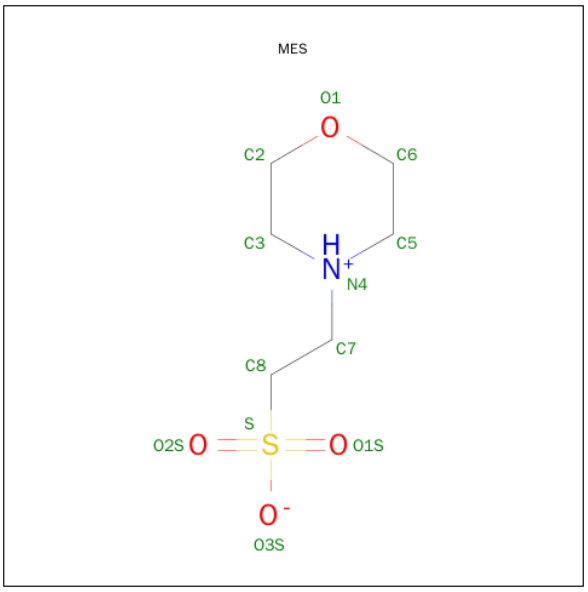
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	ASP	ENGINEERED	UNP Q68HB3
B	15	GLY	ASP	ENGINEERED	UNP Q68HB3
C	15	GLY	ASP	ENGINEERED	UNP Q68HB3
D	15	GLY	ASP	ENGINEERED	UNP Q68HB3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

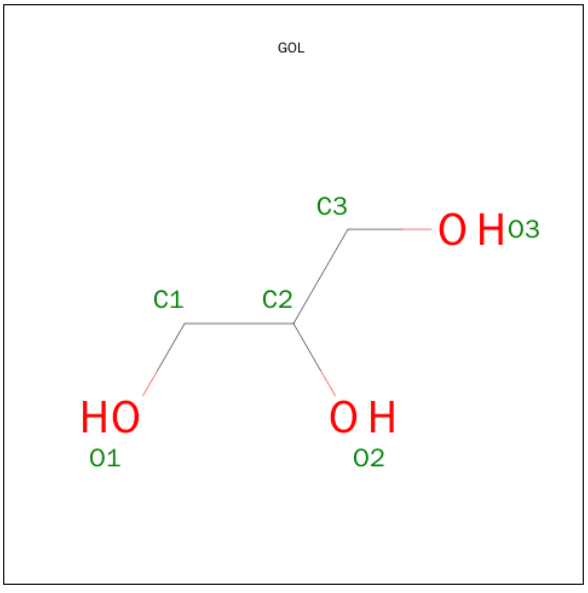
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

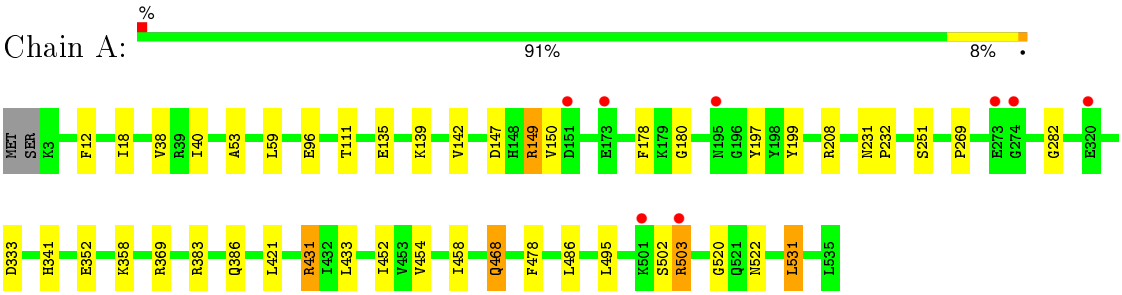
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	557	Total O 557 557	0	0
5	B	584	Total O 584 584	0	0
5	C	403	Total O 403 403	0	0
5	D	543	Total O 543 543	0	0

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.

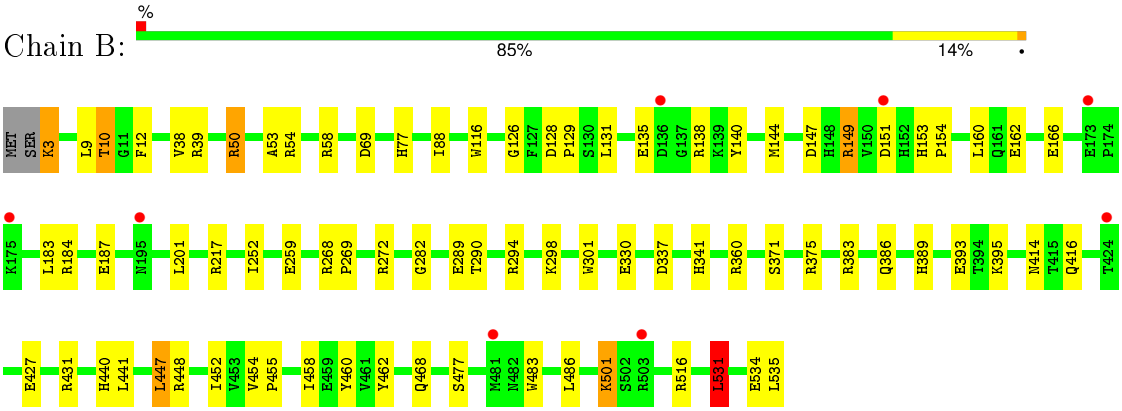
- Molecule 1: beta-D-xylosidase

Chain A:



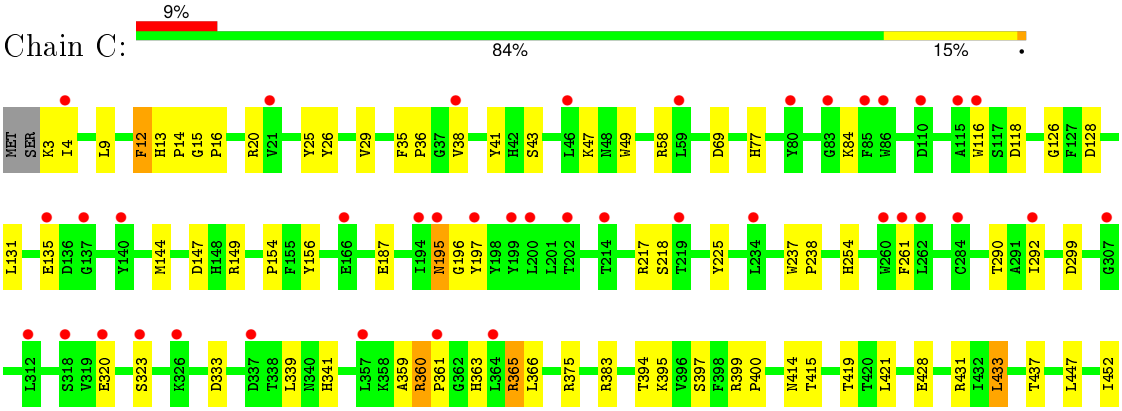
- Molecule 1: beta-D-xylosidase

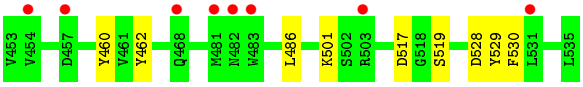
Chain B:



- Molecule 1: beta-D-xylosidase

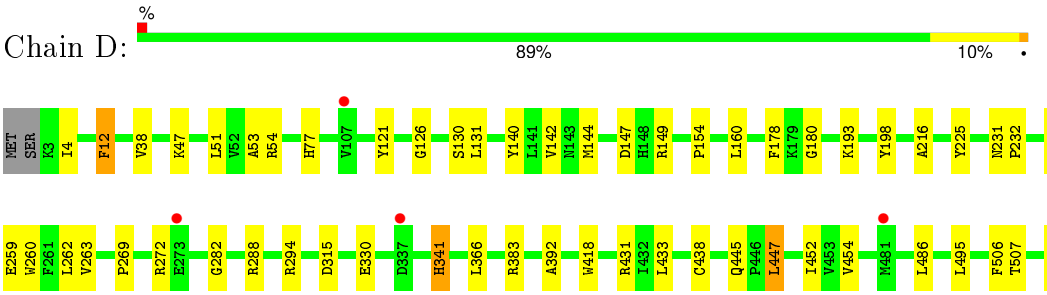
Chain C:





• Molecule 1: beta-D-xylosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.18Å 140.18Å 232.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 20.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.15) 99.6 (20.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.276 0.200 , 0.281	Depositor DCC
R_{free} test set	6301 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 125972 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19639	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, 0.375 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: GOL, CA, MES

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	0.44	0/4516	0.59	1/6154 (0.0%)
1	B	0.45	0/4516	0.60	1/6154 (0.0%)
1	C	0.41	0/4516	0.56	0/6154
1	D	0.45	0/4516	0.58	0/6154
All	All	0.44	0/18064	0.59	2/24616 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	531	LEU	CA-CB-CG	7.59	132.76	115.30
1	B	531	LEU	CA-CB-CG	7.03	131.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4372	0	4162	24	0
1	B	4372	0	4162	53	0
1	C	4372	0	4162	53	0
1	D	4372	0	4162	36	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	3	0
3	D	12	0	12	4	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	557	0	0	5	0
5	B	584	0	0	6	0
5	C	403	0	0	13	0
5	D	543	0	0	2	0
All	All	19639	0	16716	163	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 (163) 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:50:ARG:HH11	1:B:50:ARG:HG2	1.22	1.02
1:B:50:ARG:HH11	1:B:50:ARG:CG	1.87	0.87
1:B:54:ARG:HE	3:B:3006:MES:H82	1.43	0.84
1:C:197:TYR:HB3	5:C:3298:HOH:O	1.79	0.81
1:B:3:LYS:HE3	5:B:3073:HOH:O	1.81	0.79
1:C:58:ARG:NH2	1:C:116:TRP:O	2.19	0.76
1:A:111:THR:HG21	5:A:3038:HOH:O	1.83	0.76
1:B:50:ARG:HG2	1:B:50:ARG:NH1	1.99	0.75
1:C:195:ASN:HD22	1:C:196:GLY:H	1.35	0.72
1:B:138:ARG:HD2	1:B:162:GLU:OE2	1.90	0.71
1:A:369:ARG:NH2	1:A:522:ASN:OD1	2.23	0.70
1:B:259:GLU:OE1	1:B:294:ARG:NH2	2.26	0.69
1:B:53:ALA:HA	3:B:3006:MES:H51	1.73	0.69
1:C:147:ASP:OD1	1:C:149:ARG:HD3	1.94	0.68
1:D:147:ASP:OD1	1:D:149:ARG:HD3	1.96	0.66
1:D:447:LEU:HD21	1:D:486:LEU:HD22	1.78	0.65
1:D:53:ALA:HA	3:D:3007:MES:H82	1.77	0.65
1:C:375:ARG:CZ	5:C:3223:HOH:O	2.45	0.65
1:C:419:THR:HG22	1:C:437:THR:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:ARG:HD2	5:D:3031:HOH:O	1.98	0.63
1:C:4:ILE:HG12	1:C:47:LYS:HB2	1.80	0.62
1:C:394:THR:HB	5:C:3114:HOH:O	1.98	0.62
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.14	0.62
1:C:58:ARG:NH1	1:C:118:ASP:OD1	2.32	0.62
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.82	0.62
1:B:10:THR:HG22	1:B:386:GLN:HB3	1.81	0.61
1:B:10:THR:HG23	1:B:386:GLN:O	2.00	0.61
1:D:140:TYR:HB3	1:D:160:LEU:HD11	1.83	0.61
1:A:383:ARG:NH2	1:A:386:GLN:OE1	2.34	0.60
1:C:135:GLU:HG2	5:C:3251:HOH:O	2.01	0.60
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.37	0.60
1:D:433:LEU:HB2	1:D:452:ILE:HB	1.83	0.60
1:D:53:ALA:HA	3:D:3007:MES:C8	2.33	0.59
1:B:9:LEU:HB2	1:B:290:THR:HB	1.85	0.58
1:C:77:HIS:CD2	1:C:131:LEU:H	2.20	0.58
1:C:433:LEU:HB3	1:C:452:ILE:HB	1.85	0.58
1:C:339:LEU:O	5:C:3411:HOH:O	2.17	0.58
1:A:147:ASP:OD1	1:A:149:ARG:HD2	2.04	0.57
1:A:433:LEU:HB2	1:A:452:ILE:HB	1.87	0.57
1:D:77:HIS:CD2	1:D:131:LEU:H	2.22	0.57
1:C:20:ARG:HD3	1:C:254:HIS:O	2.05	0.56
1:C:399:ARG:NH2	5:C:3343:HOH:O	2.37	0.56
1:D:126:GLY:HA3	1:D:144:MET:O	2.05	0.56
1:B:10:THR:CG2	1:B:386:GLN:O	2.53	0.56
1:B:50:ARG:NH1	1:B:50:ARG:CG	2.59	0.56
1:B:416:GLN:HG2	1:B:441:LEU:HD13	1.88	0.56
1:C:195:ASN:HD22	1:C:196:GLY:N	2.03	0.55
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.87	0.55
1:C:26:TYR:HA	1:C:41:TYR:O	2.07	0.55
1:C:195:ASN:ND2	1:C:196:GLY:H	2.05	0.55
1:D:142:VAL:HG13	1:D:160:LEU:HD13	1.89	0.54
1:C:421:LEU:HD13	1:C:486:LEU:HD13	1.90	0.54
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.43	0.53
1:B:140:TYR:HB3	1:B:160:LEU:HD11	1.91	0.53
1:D:294:ARG:NH1	1:D:315:ASP:O	2.37	0.53
1:C:126:GLY:HA3	1:C:144:MET:O	2.08	0.53
1:D:431:ARG:HD3	1:D:454:VAL:HB	1.90	0.52
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.90	0.52
1:B:88:ILE:HG21	1:B:129:PRO:HB2	1.92	0.52
1:A:458:ILE:HD12	1:A:478:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD13	1:A:486:LEU:CD1	2.41	0.51
1:C:359:ALA:HB3	1:C:365:ARG:HG3	1.93	0.50
1:C:421:LEU:HD13	1:C:486:LEU:CD1	2.42	0.50
1:C:43:SER:HB2	1:C:49:TRP:CE3	2.47	0.50
1:C:156:TYR:O	5:C:3402:HOH:O	2.19	0.50
1:A:231:ASN:CG	1:A:232:PRO:HA	2.32	0.49
1:D:272:ARG:HD2	5:D:3407:HOH:O	2.11	0.49
1:B:166:GLU:HB2	5:B:3376:HOH:O	2.13	0.49
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.94	0.49
1:B:371:SER:HA	1:B:516:ARG:HD3	1.95	0.49
1:B:393:GLU:HB3	1:B:531:LEU:HG	1.95	0.48
1:B:147:ASP:OD1	1:B:149:ARG:HD3	2.14	0.48
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.61	0.48
1:B:77:HIS:CD2	1:B:131:LEU:H	2.31	0.48
1:B:389:HIS:HB2	1:B:535:LEU:HD12	1.96	0.47
1:C:395:LYS:HD2	1:C:462:TYR:CE1	2.49	0.47
1:A:111:THR:HG22	5:A:3278:HOH:O	2.13	0.47
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.14	0.47
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.63	0.47
1:B:58:ARG:NH2	1:B:116:TRP:O	2.48	0.47
1:B:128:ASP:N	1:B:129:PRO:CD	2.78	0.47
1:A:520:GLY:HA3	1:D:121:TYR:OH	2.14	0.47
1:C:363:HIS:CE1	5:C:3355:HOH:O	2.68	0.47
1:A:421:LEU:HD13	1:A:486:LEU:HD11	1.97	0.46
1:D:53:ALA:CA	3:D:3007:MES:H82	2.45	0.46
1:C:217:ARG:HB2	5:C:3298:HOH:O	2.15	0.46
1:C:20:ARG:HG3	1:C:25:TYR:CE1	2.50	0.46
1:D:231:ASN:CG	1:D:232:PRO:HA	2.36	0.45
1:C:116:TRP:HB2	5:C:3191:HOH:O	2.15	0.45
1:B:272:ARG:HD2	5:B:3235:HOH:O	2.16	0.45
1:C:395:LYS:HB3	1:C:528:ASP:HB3	1.99	0.45
1:B:54:ARG:NE	3:B:3006:MES:H82	2.22	0.45
1:C:530:PHE:HD1	5:C:3114:HOH:O	2.00	0.45
1:B:427:GLU:OE1	1:C:149:ARG:NH2	2.47	0.45
1:D:330:GLU:O	1:D:531:LEU:HA	2.17	0.45
1:B:452:ILE:HD12	1:B:452:ILE:N	2.32	0.45
1:A:468:GLN:HG3	5:A:3152:HOH:O	2.17	0.45
1:D:51:LEU:HD23	1:D:341:HIS:CG	2.52	0.45
1:B:375:ARG:HE	1:B:375:ARG:HB2	1.52	0.44
1:D:250:ALA:HB1	1:D:262:LEU:HG	1.99	0.44
1:D:130:SER:HB3	1:D:142:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ALA:HB1	1:D:225:TYR:HB3	1.98	0.44
1:C:360:ARG:HA	1:C:361:PRO:HD2	1.82	0.44
1:B:10:THR:CG2	1:B:386:GLN:HB3	2.48	0.44
1:D:250:ALA:HA	1:D:263:VAL:O	2.17	0.44
1:A:352:GLU:OE1	1:A:358:LYS:HD2	2.17	0.44
1:C:15:GLY:N	1:C:16:PRO:HD3	2.33	0.44
1:C:147:ASP:O	1:C:154:PRO:HA	2.18	0.44
1:B:147:ASP:O	1:B:154:PRO:HA	2.18	0.44
1:B:217:ARG:HG2	1:B:301:TRP:CH2	2.53	0.43
1:D:193:LYS:HD3	1:D:198:TYR:CE1	2.53	0.43
1:D:54:ARG:HH21	3:D:3007:MES:H72	1.84	0.43
1:B:447:LEU:HD21	1:B:486:LEU:HD22	1.99	0.43
1:B:184:ARG:HD2	5:B:3096:HOH:O	2.19	0.43
1:A:383:ARG:HD2	5:A:3118:HOH:O	2.18	0.43
1:C:394:THR:CB	5:C:3114:HOH:O	2.61	0.43
1:B:69:ASP:CG	1:B:414:ASN:HB2	2.39	0.43
1:D:418:TRP:CZ2	1:D:438:CYS:HB2	2.54	0.43
1:C:35:PHE:CG	1:C:36:PRO:HA	2.54	0.43
1:B:431:ARG:HD3	1:B:454:VAL:HB	2.01	0.43
1:C:12:PHE:CD1	1:C:14:PRO:HD3	2.54	0.43
1:B:395:LYS:HE2	1:B:460:TYR:CG	2.54	0.43
1:D:147:ASP:O	1:D:154:PRO:HA	2.19	0.42
1:B:330:GLU:O	1:B:531:LEU:HB2	2.19	0.42
1:A:269:PRO:HB3	1:A:282:GLY:HA3	2.01	0.42
1:B:534:GLU:HG2	1:B:535:LEU:HD13	2.02	0.42
1:B:298:LYS:HE3	1:B:298:LYS:HB2	1.77	0.42
1:A:208:ARG:NH2	1:A:503:ARG:HG3	2.33	0.42
1:B:126:GLY:HA3	1:B:144:MET:O	2.19	0.42
1:C:218:SER:HB2	1:C:225:TYR:HA	2.01	0.42
1:D:254:HIS:HB2	1:D:260:TRP:CZ3	2.54	0.42
1:A:18:ILE:HG22	1:A:251:SER:OG	2.19	0.42
1:A:197:TYR:HB2	1:A:199:TYR:CE1	2.54	0.42
1:C:323:SER:HB2	5:C:3190:HOH:O	2.18	0.42
1:D:178:PHE:CE2	1:D:180:GLY:HA2	2.55	0.42
1:D:269:PRO:HB3	1:D:282:GLY:HA3	2.02	0.42
1:A:142:VAL:HG22	5:A:3546:HOH:O	2.19	0.42
1:A:96:GLU:OE2	1:A:502:SER:HB2	2.20	0.41
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.40	0.41
1:C:237:TRP:HB3	1:C:238:PRO:HD3	2.02	0.41
1:C:77:HIS:HD2	1:C:131:LEU:H	1.64	0.41
1:C:9:LEU:HB2	1:C:290:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:SER:HB2	1:C:460:TYR:CE1	2.55	0.41
1:B:201:LEU:HD22	1:B:252:ILE:HG13	2.01	0.41
1:C:375:ARG:HG2	1:C:415:THR:HG21	2.02	0.41
1:B:153:HIS:HA	1:B:154:PRO:HD3	1.90	0.41
1:D:392:ALA:HA	1:D:531:LEU:O	2.21	0.41
1:A:150:VAL:HG23	1:D:445:GLN:OE1	2.21	0.41
1:C:13:HIS:HD2	1:C:29:VAL:HG21	1.86	0.41
1:B:39:ARG:NH2	5:B:3584:HOH:O	2.14	0.41
1:B:128:ASP:OD2	1:B:187:GLU:HG2	2.20	0.41
1:B:440:HIS:NE2	1:B:501:LYS:HD3	2.35	0.41
1:C:517:ASP:OD1	1:C:519:SER:OG	2.22	0.41
1:A:40:ILE:HB	1:A:53:ALA:HB3	2.03	0.41
1:B:468:GLN:NE2	5:B:3375:HOH:O	2.54	0.41
1:D:12:PHE:CE1	1:D:507:THR:HA	2.56	0.41
1:B:455:PRO:HB2	1:B:458:ILE:HG12	2.02	0.41
1:C:261:PHE:HB3	1:C:292:ILE:HD11	2.02	0.41
1:D:259:GLU:OE1	1:D:294:ARG:NH2	2.54	0.40
1:C:128:ASP:OD2	1:C:187:GLU:HB2	2.21	0.40
1:C:395:LYS:HB2	1:C:529:TYR:CE2	2.57	0.40
1:B:462:TYR:HB3	1:B:483:TRP:CH2	2.56	0.40
1:B:462:TYR:HB2	1:B:477:SER:HB3	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	531/535 (99%)	501 (94%)	28 (5%)	2 (0%)	39	34
1	B	531/535 (99%)	505 (95%)	24 (4%)	2 (0%)	39	34
1	C	531/535 (99%)	492 (93%)	37 (7%)	2 (0%)	39	34
1	D	531/535 (99%)	504 (95%)	25 (5%)	2 (0%)	39	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2124/2140 (99%)	2002 (94%)	114 (5%)	8 (0%)	39 34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	38	VAL
1	B	12	PHE
1	B	38	VAL
1	C	38	VAL
1	D	12	PHE
1	D	38	VAL
1	C	12	PHE

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	468/470 (100%)	457 (98%)	11 (2%)	57 60
1	B	468/470 (100%)	453 (97%)	15 (3%)	46 45
1	C	468/470 (100%)	453 (97%)	15 (3%)	46 45
1	D	468/470 (100%)	463 (99%)	5 (1%)	80 85
All	All	1872/1880 (100%)	1826 (98%)	46 (2%)	55 58

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	135	GLU
1	A	139	LYS
1	A	149	ARG
1	A	333	ASP
1	A	341	HIS
1	A	431	ARG

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Mol	Chain	Res	Type
1	A	468	GLN
1	A	495	LEU
1	A	503	ARG
1	A	531	LEU
1	B	3	LYS
1	B	10	THR
1	B	50	ARG
1	B	135	GLU
1	B	149	ARG
1	B	151	ASP
1	B	183	LEU
1	B	337	ASP
1	B	341	HIS
1	B	360	ARG
1	B	383	ARG
1	B	447	LEU
1	B	448	ARG
1	B	501	LYS
1	B	531	LEU
1	C	3	LYS
1	C	84	LYS
1	C	195	ASN
1	C	299	ASP
1	C	320	GLU
1	C	333	ASP
1	C	341	HIS
1	C	360	ARG
1	C	365	ARG
1	C	366	LEU
1	C	383	ARG
1	C	428	GLU
1	C	433	LEU
1	C	447	LEU
1	C	501	LYS
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	447	LEU
1	D	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	249	HIS
1	A	280	HIS
1	A	422	GLN
1	B	77	HIS
1	C	77	HIS
1	C	195	ASN
1	C	422	GLN
1	D	77	HIS
1	D	422	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

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	MES	A	3005	-	11,12,12	1.12	1 (9%)	14,16,16	6.82	8 (57%)
4	GOL	A	3008	-	5,5,5	0.37	0	5,5,5	0.68	0
3	MES	B	3006	-	11,12,12	1.23	2 (18%)	14,16,16	7.35	7 (50%)
4	GOL	B	3009	-	5,5,5	0.35	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	C	3010	-	5,5,5	0.37	0	5,5,5	0.18	0
3	MES	D	3007	-	11,12,12	6.35	3 (27%)	14,16,16	7.19	7 (50%)
4	GOL	D	3011	-	5,5,5	0.36	0	5,5,5	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	3005	-	-	0/6/14/14	0/1/1/1
4	GOL	A	3008	-	-	0/4/4/4	0/0/0/0
3	MES	B	3006	-	-	0/6/14/14	0/1/1/1
4	GOL	B	3009	-	-	0/4/4/4	0/0/0/0
4	GOL	C	3010	-	-	0/4/4/4	0/0/0/0
3	MES	D	3007	-	-	0/6/14/14	0/1/1/1
4	GOL	D	3011	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3006	MES	O2S-S	2.03	1.51	1.45
3	A	3005	MES	O1S-S	2.18	1.52	1.45
3	B	3006	MES	O1S-S	2.41	1.52	1.45
3	D	3007	MES	O1S-S	9.92	1.76	1.45
3	D	3007	MES	O2S-S	10.25	1.77	1.45
3	D	3007	MES	O3S-S	15.21	1.85	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3007	MES	O3S-S-O2S	-19.84	65.43	111.61
3	B	3006	MES	O3S-S-O2S	-12.38	82.79	111.61
3	D	3007	MES	O3S-S-O1S	-12.13	83.39	111.61
3	A	3005	MES	O3S-S-O2S	-12.12	83.40	111.61
3	B	3006	MES	O3S-S-O1S	-11.69	84.40	111.61
3	A	3005	MES	O3S-S-O1S	-11.53	84.78	111.61
3	D	3007	MES	C7-N4-C5	2.45	117.55	111.27
3	A	3005	MES	O2S-S-O1S	2.46	122.43	113.48
3	A	3005	MES	C7-N4-C3	2.68	118.13	111.27
3	B	3006	MES	C7-N4-C3	3.05	119.08	111.27
3	A	3005	MES	C7-N4-C5	3.21	119.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3007	MES	C7-N4-C3	3.47	120.17	111.27
3	D	3007	MES	O2S-S-O1S	3.59	126.54	113.48
3	B	3006	MES	C7-N4-C5	3.86	121.16	111.27
3	B	3006	MES	C5-N4-C3	5.00	119.73	108.90
3	D	3007	MES	C5-N4-C3	6.16	122.25	108.90
3	A	3005	MES	C5-N4-C3	6.22	122.36	108.90
3	D	3007	MES	O2S-S-C8	10.08	115.50	106.91
3	A	3005	MES	O1S-S-C8	12.33	117.43	106.91
3	A	3005	MES	O2S-S-C8	12.40	117.49	106.91
3	B	3006	MES	O1S-S-C8	13.34	118.28	106.91
3	B	3006	MES	O2S-S-C8	15.16	119.84	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3006	MES	3	0
3	D	3007	MES	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^{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	533/535 (99%)	-0.06	8 (1%) 76 82	13, 27, 41, 50	0
1	B	533/535 (99%)	-0.13	8 (1%) 76 82	13, 26, 40, 46	0
1	C	533/535 (99%)	0.76	48 (9%) 12 18	22, 42, 55, 64	0
1	D	533/535 (99%)	-0.07	4 (0%) 87 90	14, 27, 41, 46	0
All	All	2132/2140 (99%)	0.12	68 (3%) 51 61	13, 30, 50, 64	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	483	TRP	4.8
1	B	151	ASP	4.5
1	C	481	MET	4.4
1	A	151	ASP	4.3
1	C	482	ASN	3.7
1	C	135	GLU	3.5
1	C	323	SER	3.4
1	C	457	ASP	3.3
1	C	361	PRO	3.3
1	C	199	TYR	3.3
1	A	503	ARG	3.2
1	C	195	ASN	3.1
1	A	274	GLY	3.1
1	D	273	GLU	3.1
1	C	83	GLY	3.1
1	C	46	LEU	3.0
1	C	503	ARG	3.0
1	A	195	ASN	3.0
1	B	173	GLU	2.9
1	C	468	GLN	2.9
1	C	337	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	202	THR	2.9
1	C	318	SER	2.9
1	D	481	MET	2.9
1	C	200	LEU	2.8
1	B	503	ARG	2.8
1	C	21	VAL	2.8
1	C	260	TRP	2.7
1	C	166	GLU	2.7
1	C	312	LEU	2.6
1	C	357	LEU	2.6
1	B	195	ASN	2.5
1	C	261	PHE	2.5
1	C	364	LEU	2.5
1	A	173	GLU	2.5
1	C	38	VAL	2.4
1	A	320	GLU	2.4
1	B	481	MET	2.4
1	C	4	ILE	2.4
1	C	284	CYS	2.4
1	C	86	TRP	2.3
1	C	219	THR	2.3
1	B	175	LYS	2.3
1	D	107	VAL	2.3
1	C	320	GLU	2.2
1	C	292	ILE	2.2
1	C	137	GLY	2.2
1	C	80	TYR	2.2
1	C	140	TYR	2.2
1	C	59	LEU	2.1
1	B	424	THR	2.1
1	A	501	LYS	2.1
1	C	194	ILE	2.1
1	C	116	TRP	2.1
1	C	197	TYR	2.1
1	C	454	VAL	2.1
1	A	273	GLU	2.1
1	C	110	ASP	2.1
1	D	337	ASP	2.1
1	C	307	GLY	2.1
1	C	234	LEU	2.1
1	C	85	PHE	2.1
1	C	326	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	262	LEU	2.0
1	C	531	LEU	2.0
1	C	115	ALA	2.0
1	B	136	ASP	2.0
1	C	214	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
3	MES	D	3007	12/12	0.53	0.43	22.98	109,110,112,112	0
3	MES	B	3006	12/12	0.82	0.29	5.11	74,76,77,77	0
4	GOL	A	3008	6/6	0.92	0.13	1.48	24,25,26,26	0
3	MES	A	3005	12/12	0.97	0.13	1.39	29,34,37,37	0
4	GOL	C	3010	6/6	0.96	0.14	0.33	31,31,31,33	0
4	GOL	D	3011	6/6	0.96	0.08	-0.24	22,25,25,28	0
4	GOL	B	3009	6/6	0.94	0.10	-0.43	37,39,40,41	0
2	CA	A	3001	1/1	0.99	0.06	-1.43	25,25,25,25	0
2	CA	D	3004	1/1	0.98	0.06	-1.78	30,30,30,30	0
2	CA	B	3002	1/1	0.99	0.04	-3.32	27,27,27,27	0
2	CA	C	3003	1/1	0.86	0.09	-3.53	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.