Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:56 AM GMT

PDB ID	:	3QHN
Title	:	Crystal analysis of the complex structure, E201A-cellotetraose, of endocellulase from pyrococcus horikoshii
Authors	:	Kim, H.-W.; Ishikawa, K.
Deposited on	:	2011-01-26
Resolution	:	1.99 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:

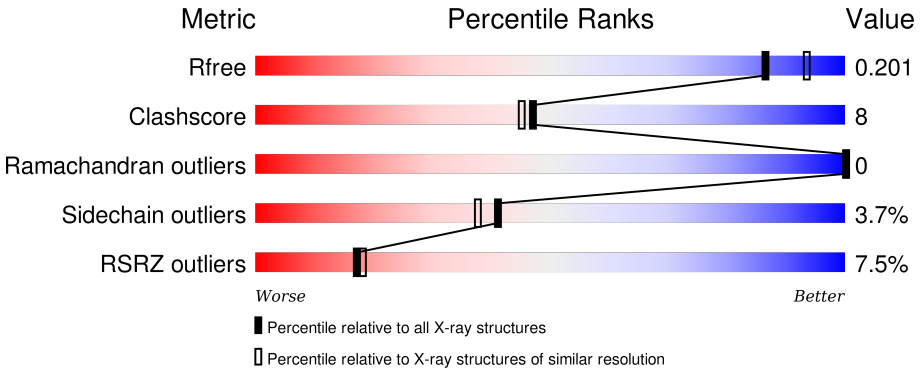
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	458	5% 67% 14% • 18%
1	B	458	2% 72% 9% • 18%
1	C	458	12% 62% 19% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9624 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.

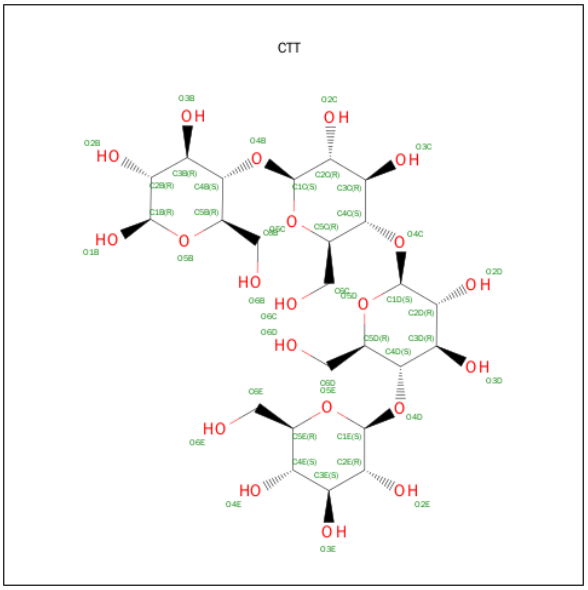
- Molecule 1 is a protein called 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	B	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			
1	C	377	Total	C	N	O	S	0	0	0
			3067	2000	502	555	10			

There are 3 discrepancies between the modelled and reference sequences:

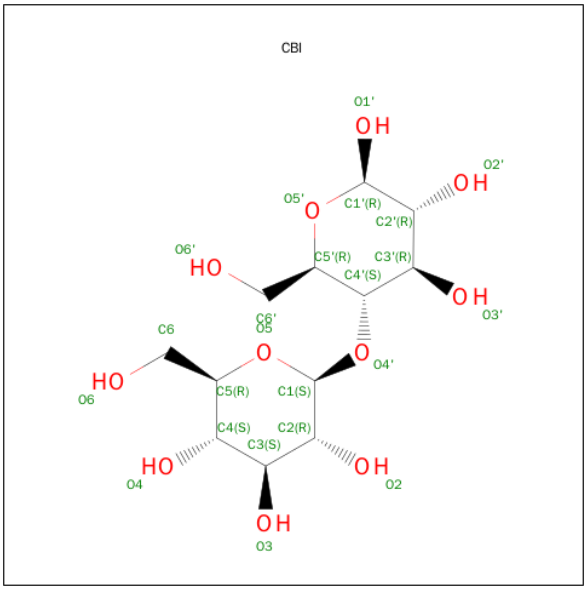
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ALA	GLU	ENGINEERED MUTATION	UNP O58925
B	201	ALA	GLU	ENGINEERED MUTATION	UNP O58925
C	201	ALA	GLU	ENGINEERED MUTATION	UNP O58925

- Molecule 2 is SUGAR (BETA-D-GLUCOPYRANOSYL-(1->4)-BETA-D-GLUCOPYRANOSYL-(1->4)-BETA-D-GLUCOPYRANOSYL-(1->4)-BETA-D-GLUCOPYRANOSE) (three-letter code: CTT) (formula: $C_{24}H_{42}O_{21}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 45 24 21	0	0
2	B	1	Total C O 45 24 21	0	0
2	C	1	Total C O 45 24 21	0	0

- Molecule 3 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 23 12 11	0	0

- Molecule 4 is water.

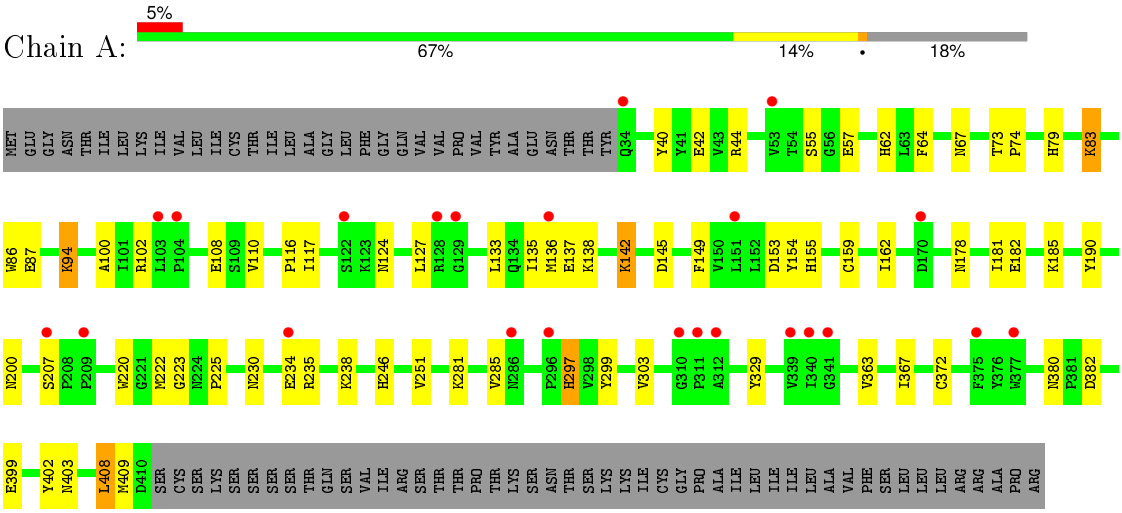
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	108	Total O 108 108	0	0
4	B	106	Total O 106 106	0	0
4	C	51	Total O 51 51	0	0

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.

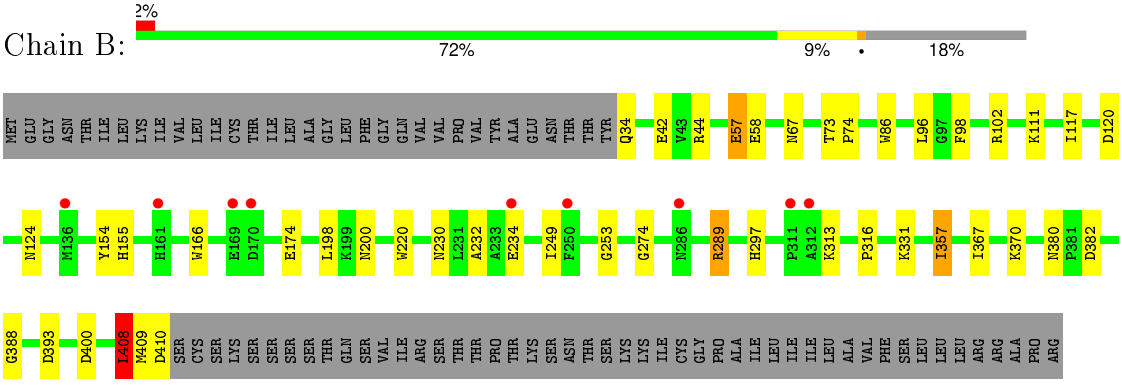
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain A:



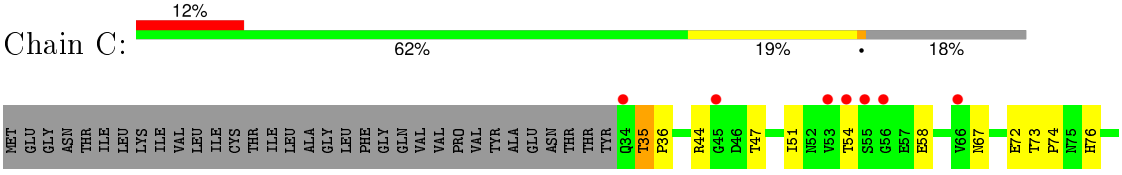
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

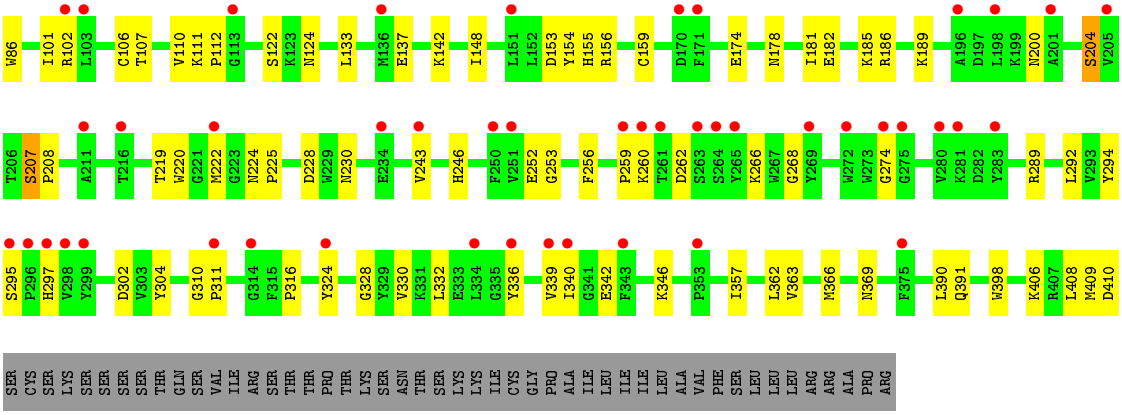
Chain B:



- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain C:




W86 I101 R102 L103 C106 T107 V110 K111 P112 G113 S122 K123 N124 L133 M136 E137 K142 I148 L151 L152 D153 Y154 H155 R156 C159 D170 F171 E174 N178 I181 E182 K185 R186 K189 A196 D197 L198 K199 N200 A201 S204 V205
T206 S207 P208 A211 T216 T219 W220 G221 N222 G223 N224 P225 D228 W229 N230 E234 V243 H246 F250 V251 E252 G253 F256 P259 K260 T261 D262 S263 S264 Y265 K266 W267 G268 Y269 W272 W273 G274 G275 V280 K281 D282 Y283 R289 L292 V293 Y294
S295 P296 H297 V298 Y299 D302 V303 Y304 G310 P311 G314 F315 P316 Y324 G328 Y329 V330 K331 L332 E333 L334 G335 Y336 V339 I340 G341 E342 F343 K346 P353 I357 L362 V363 M366 N369 F375 L390 Q391 W398 K406 R407 L408 M409 D410
SER CYS SER LYS SER SER SER SER THR GLN SER VAL ILE ARG SER THR THR PRO THR LYS SER ASN THR SER LYS LYS ILE CYS GLY PRO ALA ILE LEU ILE ILE LEU ALA VAL PHE SER LEU LEU LEU ARG ARG ALA PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.32Å 58.35Å 138.27Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	28.99 – 1.99 28.99 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.8 (28.99-1.99) 90.8 (28.99-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.248 0.198 , 0.201	Depositor DCC
R_{free} test set	3988 reflections (5.50%)	DCC
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 79673 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9624	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CTT, CBI

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	1.07	2/3178 (0.1%)	0.87	2/4339 (0.0%)
1	B	1.12	3/3178 (0.1%)	0.92	5/4339 (0.1%)
1	C	0.88	0/3178	0.80	1/4339 (0.0%)
All	All	1.03	5/9534 (0.1%)	0.87	8/13017 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CG-CD	-6.25	1.42	1.51
1	B	98	PHE	CE1-CZ	5.64	1.48	1.37
1	A	402	TYR	CG-CD1	5.36	1.46	1.39
1	B	174	GLU	CG-CD	5.21	1.59	1.51
1	A	329	TYR	CE1-CZ	5.21	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	400	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	289	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	393	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	235	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	408	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	153	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	390	LEU	CB-CG-CD1	-5.09	102.34	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3067	0	2907	42	0
1	B	3067	0	2907	30	1
1	C	3067	0	2907	60	0
2	A	45	0	42	1	0
2	B	45	0	42	4	0
2	C	45	0	42	2	1
3	C	23	0	22	2	0
4	A	108	0	0	1	0
4	B	106	0	0	0	0
4	C	51	0	0	0	0
All	All	9624	0	8869	137	1

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 8.

All (137) 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:316:PRO:HG3	1:B:357:ILE:CD1	1.87	1.04
1:B:316:PRO:HG3	1:B:357:ILE:HD13	1.53	0.89
1:C:266:LYS:H	1:C:266:LYS:HD2	1.34	0.89
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.24	0.86
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.29	0.80
1:C:35:THR:HB	1:C:246:HIS:HB3	1.68	0.76
1:C:181:ILE:HG22	1:C:185:LYS:HE3	1.69	0.74
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.51	0.72
1:A:55:SER:OG	1:A:57:GLU:HG3	1.90	0.72
1:C:266:LYS:H	1:C:266:LYS:CD	2.03	0.71
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.38	0.71
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.40	0.69
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.41	0.69
1:C:200:ASN:ND2	1:C:297:HIS:HE1	1.91	0.68
1:C:200:ASN:HD21	1:C:297:HIS:HE1	1.40	0.68
1:C:266:LYS:N	1:C:266:LYS:HD2	2.10	0.66
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PRO:CG	1:B:357:ILE:CD1	2.71	0.65
1:A:133:LEU:O	1:A:137:GLU:HG3	1.97	0.64
1:B:102:ARG:HH22	1:B:200:ASN:ND2	1.95	0.64
1:B:67:ASN:ND2	1:B:102:ARG:HH11	1.95	0.64
1:B:316:PRO:HB3	1:B:357:ILE:HD11	1.80	0.64
1:B:331:LYS:HE3	1:B:370:LYS:O	1.98	0.63
1:C:362:LEU:O	1:C:366:MET:HG3	1.99	0.63
1:B:316:PRO:HG3	1:B:357:ILE:HD11	1.77	0.63
1:C:178:ASN:O	1:C:182:GLU:HG3	1.98	0.63
1:C:107:THR:HG22	1:C:111:LYS:HE3	1.81	0.62
1:A:83:LYS:HD3	1:A:83:LYS:O	1.99	0.62
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.49	0.61
1:C:342:GLU:OE1	2:C:2739:CTT:H1B	2.00	0.60
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.97	0.60
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.83	0.60
1:C:137:GLU:OE2	1:C:186:ARG:HD3	2.03	0.58
1:A:116:PRO:O	1:A:117:ILE:HD13	2.03	0.58
1:C:302:ASP:OD2	1:C:346:LYS:HB2	2.04	0.57
1:A:299:TYR:CD1	1:A:303:VAL:HG21	2.39	0.57
1:C:406:LYS:HA	1:C:409:MET:CE	2.35	0.56
1:C:292:LEU:HD21	1:C:294:TYR:CZ	2.39	0.56
1:B:316:PRO:CG	1:B:357:ILE:HD11	2.34	0.56
1:C:406:LYS:HA	1:C:409:MET:HE3	1.88	0.56
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.54	0.55
1:C:204:SER:HG	1:C:256:PHE:HD2	1.53	0.55
1:A:363:VAL:HG13	1:A:408:LEU:HD13	1.88	0.55
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.89	0.54
2:B:2739:CTT:H1E	2:B:2739:CTT:H6D	1.90	0.53
1:A:155:HIS:HA	1:A:200:ASN:CB	2.38	0.52
1:A:67:ASN:ND2	1:A:102:ARG:HH11	2.06	0.52
1:B:253:GLY:O	1:B:274:GLY:HA2	2.09	0.52
1:C:72:GLU:O	1:C:156:ARG:HD2	2.09	0.52
1:A:297:HIS:ND1	4:A:565:HOH:O	2.24	0.51
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.11	0.51
1:A:155:HIS:HA	1:A:200:ASN:HB3	1.93	0.51
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.09	0.50
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.11	0.50
1:C:86:TRP:HD1	1:C:124:ASN:ND2	2.09	0.50
3:C:459:CBI:O4	2:C:2739:CTT:H6B	2.11	0.50
1:B:316:PRO:CB	1:B:357:ILE:HD11	2.40	0.50
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLY:O	1:A:225:PRO:HD3	2.12	0.50
1:C:207:SER:HB3	1:C:208:PRO:HD2	1.93	0.49
1:A:62:HIS:CD2	1:A:372:CYS:SG	3.06	0.49
1:B:230:ASN:O	1:B:234:GLU:HG3	2.12	0.49
1:C:252:GLU:HA	1:C:295:SER:O	2.12	0.49
1:C:316:PRO:HG3	1:C:357:ILE:CG2	2.42	0.49
1:C:391:GLN:HG2	1:C:398:TRP:CE2	2.47	0.49
1:C:106:CYS:HA	1:C:156:ARG:O	2.13	0.48
1:B:367:ILE:HG13	1:B:408:LEU:CD1	2.44	0.48
1:A:162:ILE:HD11	2:A:2739:CTT:H2D	1.94	0.48
1:A:110:VAL:HA	1:A:133:LEU:HD13	1.95	0.48
1:C:51:ILE:HG12	1:C:58:GLU:HB2	1.96	0.47
1:C:406:LYS:O	1:C:410:ASP:N	2.47	0.47
1:A:73:THR:HB	1:A:74:PRO:HD2	1.97	0.47
1:C:222:MET:SD	1:C:259:PRO:HD3	2.55	0.47
1:A:94:LYS:O	1:A:94:LYS:HE3	2.15	0.47
1:B:155:HIS:HA	1:B:200:ASN:HB3	1.97	0.47
2:B:2739:CTT:C1E	2:B:2739:CTT:H6D	2.44	0.47
1:B:102:ARG:NH2	1:B:200:ASN:HD22	2.12	0.47
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.61	0.46
1:C:101:ILE:HD12	1:C:148:ILE:HG21	1.97	0.46
1:B:380:ASN:O	1:B:388:GLY:HA3	2.15	0.46
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.13	0.46
1:B:367:ILE:HG13	1:B:408:LEU:HD13	1.97	0.46
1:C:310:GLY:O	1:C:311:PRO:C	2.52	0.46
1:C:86:TRP:H	1:C:124:ASN:HD21	1.62	0.45
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.80	0.45
1:A:251:VAL:HG11	1:A:285:VAL:HG21	1.98	0.45
1:A:367:ILE:HG13	1:A:408:LEU:CD1	2.47	0.45
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.51	0.45
1:C:219:THR:O	1:C:228:ASP:HA	2.16	0.45
1:B:198:LEU:HD21	1:B:249:ILE:HG23	1.99	0.45
1:A:40:TYR:HA	1:A:246:HIS:HB2	1.99	0.45
1:C:44:ARG:NH1	1:C:58:GLU:OE1	2.47	0.44
2:B:2739:CTT:O2E	2:B:2739:CTT:H6D	2.17	0.44
1:C:228:ASP:HB3	1:C:230:ASN:OD1	2.17	0.44
2:B:2739:CTT:H1E	2:B:2739:CTT:C6D	2.47	0.44
1:A:87:GLU:CD	1:A:142:LYS:HE3	2.37	0.44
1:C:142:LYS:HA	1:C:142:LYS:HD3	1.84	0.44
1:A:178:ASN:O	1:A:182:GLU:HG3	2.18	0.44
1:A:67:ASN:ND2	1:A:102:ARG:HD3	2.28	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:O	1:A:145:ASP:HB2	2.18	0.43
1:C:44:ARG:HH12	1:C:58:GLU:CD	2.21	0.43
1:A:155:HIS:HA	1:A:200:ASN:HB2	2.01	0.43
1:A:42:GLU:OE1	1:A:44:ARG:CZ	2.66	0.43
1:A:64:PHE:CD2	1:A:409:MET:HG2	2.53	0.43
1:C:330:VAL:HG12	1:C:336:TYR:HB2	2.00	0.43
1:C:262:ASP:O	1:C:268:GLY:HA3	2.18	0.43
1:B:200:ASN:ND2	1:B:297:HIS:HE1	2.17	0.43
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.53	0.43
1:C:304:TYR:CD1	3:C:459:CBI:H5'	2.54	0.43
1:C:253:GLY:O	1:C:274:GLY:HA2	2.18	0.43
1:C:220:TRP:NE1	1:C:230:ASN:HB3	2.34	0.42
1:A:181:ILE:O	1:A:185:LYS:HG3	2.19	0.42
1:A:127:LEU:HD22	1:A:135:ILE:HG12	2.00	0.42
1:C:295:SER:HA	1:C:339:VAL:O	2.19	0.42
1:B:57:GLU:HG3	1:B:58:GLU:N	2.34	0.42
1:B:96:LEU:O	1:B:409:MET:HE1	2.19	0.42
1:C:73:THR:HB	1:C:74:PRO:CD	2.49	0.42
1:C:363:VAL:HG13	1:C:408:LEU:HB2	2.01	0.42
1:A:79:HIS:HB2	1:A:380:ASN:ND2	2.35	0.42
1:C:155:HIS:HA	1:C:200:ASN:HB3	2.00	0.42
1:C:181:ILE:CG2	1:C:185:LYS:HE3	2.46	0.42
1:C:58:GLU:HG2	1:C:58:GLU:O	2.18	0.42
1:A:190:TYR:N	1:A:190:TYR:CD2	2.87	0.42
1:A:86:TRP:HD1	1:A:124:ASN:ND2	2.18	0.42
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.54	0.41
1:C:406:LYS:HG3	1:C:409:MET:HE3	2.02	0.41
1:A:100:ALA:HA	1:A:149:PHE:O	2.20	0.41
1:A:142:LYS:HD3	1:A:142:LYS:HA	1.96	0.41
1:B:370:LYS:HB2	1:B:370:LYS:HE3	1.89	0.41
1:A:234:GLU:O	1:A:238:LYS:HG3	2.21	0.41
1:A:108:GLU:HB2	1:A:159:CYS:SG	2.61	0.41
1:B:120:ASP:OD1	1:B:120:ASP:C	2.60	0.41
1:C:76:HIS:HE1	1:C:159:CYS:SG	2.43	0.40
1:A:281:LYS:HE2	1:A:281:LYS:HB3	1.72	0.40
1:C:332:LEU:HD21	1:C:369:ASN:HB3	2.03	0.40
1:B:166:TRP:CZ2	1:B:232:ALA:HB2	2.56	0.40
1:B:73:THR:HB	1:B:74:PRO:CD	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:OE2	2:C:2739:CTT:O4E[4_545]	2.15	0.05

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	375/458 (82%)	362 (96%)	13 (4%)	0	100	100
1	B	375/458 (82%)	365 (97%)	10 (3%)	0	100	100
1	C	375/458 (82%)	361 (96%)	14 (4%)	0	100	100
All	All	1125/1374 (82%)	1088 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	323/395 (82%)	311 (96%)	12 (4%)	41	38
1	B	323/395 (82%)	314 (97%)	9 (3%)	51	50
1	C	323/395 (82%)	308 (95%)	15 (5%)	33	28
All	All	969/1185 (82%)	933 (96%)	36 (4%)	41	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	94	LYS
1	A	136	MET
1	A	138	LYS
1	A	142	LYS
1	A	154	TYR
1	A	207	SER
1	A	222	MET
1	A	297	HIS
1	A	399	GLU
1	A	403	ASN
1	A	408	LEU
1	B	34	GLN
1	B	111	LYS
1	B	117	ILE
1	B	154	TYR
1	B	289	ARG
1	B	313	LYS
1	B	357	ILE
1	B	408	LEU
1	B	410	ASP
1	C	35	THR
1	C	47	THR
1	C	54	THR
1	C	112	PRO
1	C	122	SER
1	C	153	ASP
1	C	154	TYR
1	C	174	GLU
1	C	189	LYS
1	C	204	SER
1	C	207	SER
1	C	243	VAL
1	C	260	LYS
1	C	289	ARG
1	C	340	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	ASN
1	A	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	200	ASN
1	A	359	GLN
1	B	34	GLN
1	B	67	ASN
1	B	124	ASN
1	B	161	HIS
1	B	200	ASN
1	B	359	GLN
1	C	34	GLN
1	C	67	ASN
1	C	76	HIS
1	C	115	GLN
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	297	HIS
1	C	359	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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CTT	A	2739	-	48,48,48	1.40	7 (14%)	71,71,71	1.52	11 (15%)
2	CTT	B	2739	-	48,48,48	1.31	7 (14%)	71,71,71	1.69	17 (23%)
2	CTT	C	2739	-	48,48,48	1.15	6 (12%)	71,71,71	1.90	14 (19%)
3	CBI	C	459	-	24,24,24	0.59	0	35,35,35	0.89	1 (2%)

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	CTT	A	2739	-	-	0/20/100/100	0/4/4/4
2	CTT	B	2739	-	-	0/20/100/100	0/4/4/4
2	CTT	C	2739	-	-	0/20/100/100	0/4/4/4
3	CBI	C	459	-	-	0/8/48/48	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2739	CTT	O5B-C1B	-2.56	1.38	1.43
2	C	2739	CTT	O5C-C1C	2.00	1.47	1.41
2	A	2739	CTT	O5D-C5D	2.01	1.49	1.44
2	A	2739	CTT	C1B-C2B	2.02	1.56	1.52
2	C	2739	CTT	O5D-C1D	2.07	1.47	1.41
2	B	2739	CTT	O4B-C4B	2.08	1.49	1.43
2	C	2739	CTT	C3E-C4E	2.17	1.58	1.52
2	A	2739	CTT	O2D-C2D	2.24	1.48	1.43
2	C	2739	CTT	O1B-C1B	2.28	1.47	1.39
2	A	2739	CTT	O4B-C1C	2.37	1.48	1.41
2	B	2739	CTT	C1B-C2B	2.38	1.57	1.52
2	C	2739	CTT	C4E-C5E	2.41	1.58	1.53
2	B	2739	CTT	C6D-C5D	2.50	1.60	1.51
2	B	2739	CTT	O1B-C1B	2.63	1.48	1.39
2	A	2739	CTT	O5E-C1E	2.64	1.48	1.41
2	B	2739	CTT	O5D-C1D	3.02	1.49	1.41
2	B	2739	CTT	O5C-C1C	3.28	1.50	1.41
2	A	2739	CTT	O4C-C1D	3.38	1.50	1.41
2	C	2739	CTT	O5B-C1B	4.09	1.50	1.43
2	A	2739	CTT	O5D-C1D	4.81	1.54	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2739	CTT	C1D-O4C-C4C	-5.95	102.47	118.01
2	C	2739	CTT	O4D-C1E-O5E	-4.85	98.41	110.68
2	C	2739	CTT	C6B-C5B-C4B	-4.73	99.49	113.25
2	C	2739	CTT	C1E-O4D-C4D	-4.36	106.61	118.01
2	C	2739	CTT	C1E-O5E-C5E	-4.18	105.62	113.75
2	C	2739	CTT	O4D-C4D-C3D	-3.98	96.90	107.17
2	B	2739	CTT	O3D-C3D-C2D	-3.71	101.98	110.34
2	B	2739	CTT	C1E-O4D-C4D	-3.59	108.62	118.01
2	A	2739	CTT	C3D-C4D-C5D	-3.29	103.39	110.84
2	B	2739	CTT	C1D-O5D-C5D	-2.97	107.98	113.75
2	A	2739	CTT	O2C-C2C-C1C	-2.92	103.62	110.02
2	B	2739	CTT	O5B-C1B-C2B	-2.82	105.30	109.80
2	B	2739	CTT	O4C-C1D-O5D	-2.68	103.89	110.68
2	C	2739	CTT	O4C-C4C-C5C	-2.59	102.51	109.32
2	C	2739	CTT	O5E-C5E-C4E	-2.56	104.87	109.68
2	A	2739	CTT	O4D-C1E-O5E	-2.55	104.23	110.68
2	B	2739	CTT	O4B-C1C-C2C	-2.52	101.96	108.10
2	C	2739	CTT	C3B-C4B-C5B	-2.41	105.39	110.84
2	A	2739	CTT	O4C-C1D-C2D	-2.36	102.37	108.10
2	B	2739	CTT	O3B-C3B-C4B	-2.35	104.32	109.87
2	B	2739	CTT	O2B-C2B-C1B	-2.33	104.69	109.82
2	B	2739	CTT	C1C-C2C-C3C	-2.29	105.46	109.97
2	B	2739	CTT	O2D-C2D-C3D	-2.27	105.22	110.34
3	C	459	CBI	C1'-O5'-C5'	-2.20	109.40	113.47
2	B	2739	CTT	O3E-C3E-C2E	-2.11	105.59	110.34
2	A	2739	CTT	O4D-C4D-C5D	-2.10	103.80	109.32
2	B	2739	CTT	O4C-C4C-C5C	-2.06	103.90	109.32
2	B	2739	CTT	O2B-C2B-C3B	2.01	114.87	110.34
2	C	2739	CTT	O5C-C5C-C6C	2.02	111.46	106.36
2	B	2739	CTT	O5B-C5B-C4B	2.14	114.28	109.75
2	A	2739	CTT	O3C-C3C-C2C	2.20	115.29	110.34
2	A	2739	CTT	O2D-C2D-C3D	2.77	116.58	110.34
2	A	2739	CTT	O5E-C5E-C4E	2.78	114.91	109.68
2	A	2739	CTT	O4B-C4B-C3B	2.79	114.37	107.17
2	A	2739	CTT	O4C-C1D-O5D	3.26	118.94	110.68
2	B	2739	CTT	C3D-C4D-C5D	3.37	118.45	110.84
2	B	2739	CTT	O5D-C1D-C2D	3.49	117.43	110.28
2	C	2739	CTT	C1B-O5B-C5B	3.50	119.95	113.47
2	C	2739	CTT	O5E-C1E-C2E	3.67	117.81	110.28
2	C	2739	CTT	C1B-C2B-C3B	3.68	115.91	110.43
2	A	2739	CTT	C1D-O5D-C5D	3.73	120.99	113.75
2	C	2739	CTT	C6E-C5E-C4E	4.36	123.77	113.02
2	C	2739	CTT	O4B-C4B-C3B	4.76	119.47	107.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2739	CTT	1	0
2	B	2739	CTT	4	0
2	C	2739	CTT	2	1
3	C	459	CBI	2	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	377/458 (82%)	0.27	23 (6%) 25 26	13, 25, 49, 56	8 (2%)
1	B	377/458 (82%)	0.09	9 (2%) 62 63	11, 22, 36, 46	10 (2%)
1	C	377/458 (82%)	0.81	53 (14%) 4 4	19, 38, 57, 64	9 (2%)
All	All	1131/1374 (82%)	0.39	85 (7%) 17 18	11, 27, 53, 64	27 (2%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	MET	6.9
1	C	136	MET	6.6
1	B	136	MET	5.6
1	C	340	ILE	5.0
1	C	54	THR	4.8
1	C	53	VAL	4.4
1	A	311	PRO	4.4
1	A	209	PRO	4.3
1	C	216	THR	4.3
1	C	205	VAL	4.2
1	C	283	TYR	4.2
1	C	334	LEU	4.1
1	B	169	GLU	4.1
1	C	260	LYS	4.0
1	C	296	PRO	4.0
1	A	122	SER	3.9
1	C	324	TYR	3.8
1	C	314	GLY	3.7
1	C	375	PHE	3.6
1	C	251	VAL	3.6
1	C	339	VAL	3.6
1	C	34	GLN	3.5
1	C	298	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	280	VAL	3.4
1	C	263	SER	3.4
1	C	261	THR	3.3
1	B	170	ASP	3.3
1	C	151	LEU	3.3
1	A	286	ASN	3.2
1	A	128	ARG	3.2
1	C	275	GLY	3.1
1	C	243	VAL	3.0
1	C	45	GLY	3.0
1	A	53	VAL	3.0
1	C	234	GLU	2.9
1	B	161	HIS	2.9
1	B	234	GLU	2.9
1	C	196	ALA	2.9
1	B	311	PRO	2.8
1	A	310	GLY	2.8
1	C	198	LEU	2.8
1	A	375	PHE	2.8
1	A	377	TRP	2.8
1	C	264	SER	2.8
1	C	201	ALA	2.7
1	B	312	ALA	2.7
1	C	259	PRO	2.7
1	C	336	TYR	2.7
1	C	56	GLY	2.6
1	A	340	ILE	2.6
1	A	234	GLU	2.6
1	C	353	PRO	2.6
1	A	341	GLY	2.6
1	C	295	SER	2.6
1	C	171	PHE	2.5
1	C	265	TYR	2.5
1	C	113	GLY	2.5
1	A	312	ALA	2.5
1	C	250	PHE	2.5
1	A	207	SER	2.5
1	A	296	PRO	2.5
1	C	311	PRO	2.5
1	C	343	PHE	2.4
1	A	151	LEU	2.4
1	C	170	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	34	GLN	2.3
1	A	170	ASP	2.3
1	C	297	HIS	2.3
1	C	269	TYR	2.3
1	B	250	PHE	2.3
1	C	274	GLY	2.2
1	C	211	ALA	2.2
1	B	286	ASN	2.2
1	C	272	TRP	2.2
1	C	281	LYS	2.2
1	A	129	GLY	2.2
1	C	102	ARG	2.2
1	C	222	MET	2.2
1	A	103	LEU	2.1
1	A	339	VAL	2.1
1	C	66	VAL	2.1
1	A	104	PRO	2.1
1	C	103	LEU	2.1
1	C	55	SER	2.0
1	C	299	TYR	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	CBI	C	459	23/23	0.75	0.18	0.68	55,70,77,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CTT	C	2739	45/45	0.88	0.14	0.07	28,38,46,47	0
2	CTT	B	2739	45/45	0.92	0.10	-0.23	21,30,35,40	0
2	CTT	A	2739	45/45	0.94	0.10	-0.44	22,29,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.