



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:27 am BST

PDB ID : 1VCH  
Title : Crystal Structure of a Phosphoribosyltransferase-related protein from *Thermus thermophilus*  
Authors : Rehse, P.H.; Tahirov, T.H.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-03-08  
Resolution : 1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

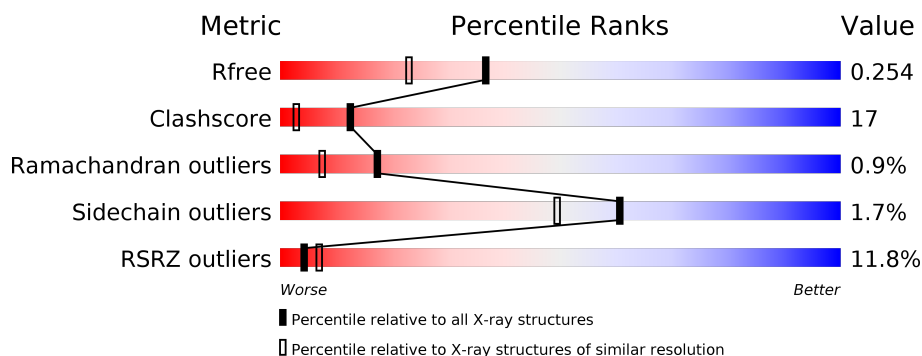
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	C	175	
1	D	175	
1	E	175	

## 2 Entry composition [i](#)

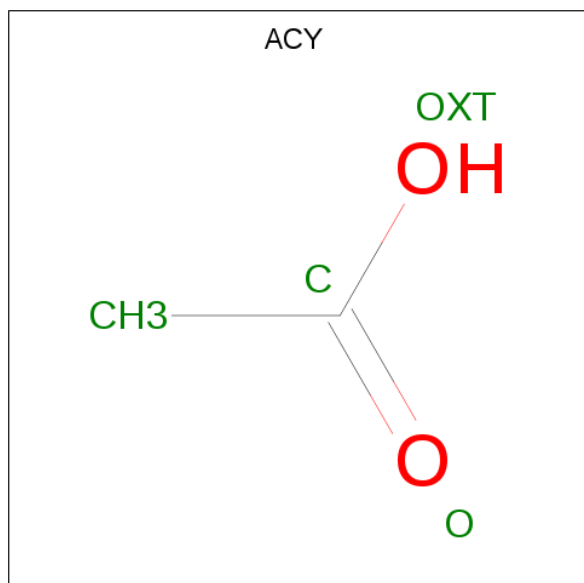
There are 5 unique types of molecules in this entry. The entry contains 6899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoribosyltransferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	1
			1317	844	234	235	4			
1	B	170	Total	C	N	O	S	0	0	0
			1327	850	236	236	5			
1	C	170	Total	C	N	O	S	0	0	1
			1322	847	235	235	5			
1	D	173	Total	C	N	O	S	0	0	0
			1349	865	239	240	5			
1	E	152	Total	C	N	O	S	0	0	0
			1189	762	216	207	4			

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

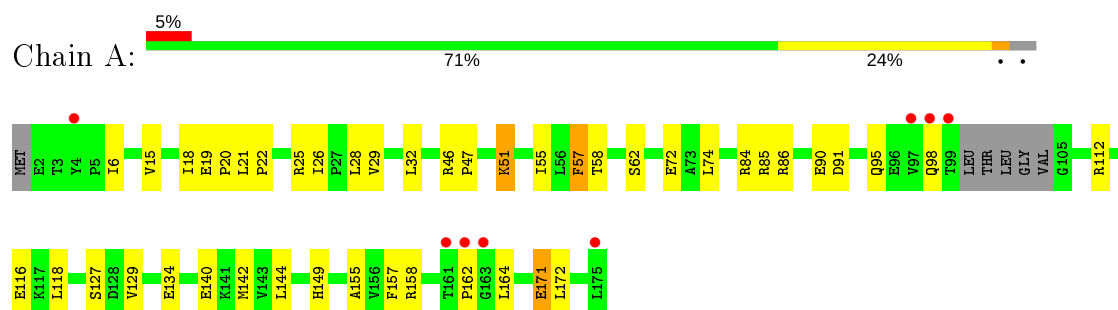
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	95	Total	O	0	0
			95	95		
5	C	81	Total	O	0	0
			81	81		
5	D	97	Total	O	0	0
			97	97		
5	E	31	Total	O	0	0
			31	31		

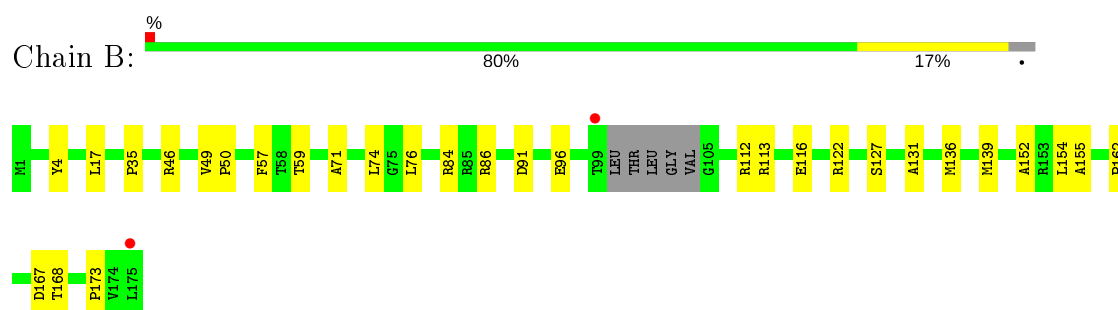
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

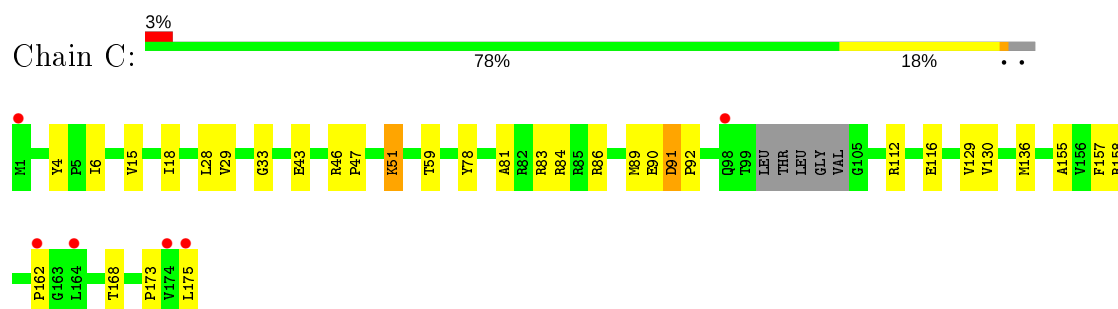
- Molecule 1: Phosphoribosyltransferase-related protein



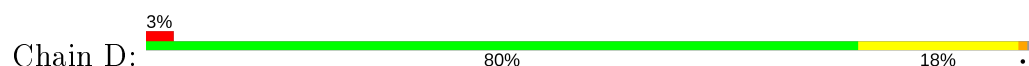
- Molecule 1: Phosphoribosyltransferase-related protein

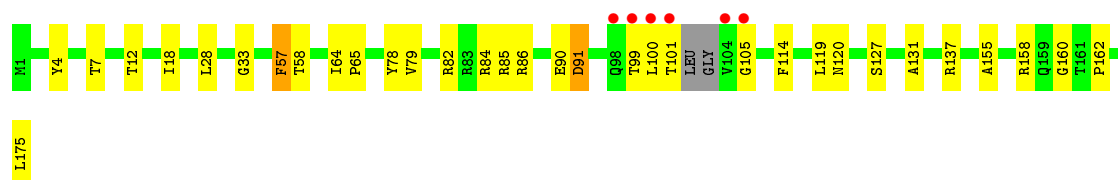


- Molecule 1: Phosphoribosyltransferase-related protein

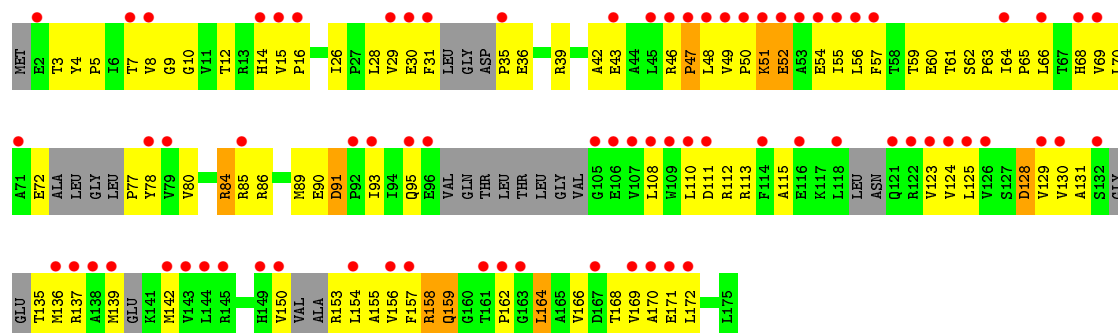


- Molecule 1: Phosphoribosyltransferase-related protein





- Molecule 1: Phosphoribosyltransferase-related protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.42Å 61.41Å 102.39Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	44.98 – 1.94 44.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.98-1.94) 94.2 (44.98-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.259 0.227 , 0.254	Depositor DCC
$R_{free}$ test set	4057 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACY, CL

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	0.32	0/1343	0.62	0/1829
1	B	0.34	0/1353	0.63	0/1842
1	C	0.32	0/1348	0.62	0/1834
1	D	0.30	0/1375	0.63	0/1873
1	E	0.38	0/1208	0.78	2/1634 (0.1%)
All	All	0.33	0/6627	0.66	2/9012 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	52	GLU	N-CA-C	-7.53	90.68	111.00
1	E	84	ARG	NE-CZ-NH2	6.68	123.64	120.30

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	1317	0	1372	43	0
1	B	1327	0	1386	20	0
1	C	1322	0	1378	31	0
1	D	1349	0	1413	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1189	0	1224	112	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	C	1	0	0	0	0
5	A	69	0	0	2	0
5	B	95	0	0	2	0
5	C	81	0	0	1	0
5	D	97	0	0	4	0
5	E	31	0	0	2	0
All	All	6899	0	6785	223	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 17.

All (223) 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:E:57:PHE:HE2	1:E:139:MET:HB3	1.14	1.09
1:E:95:GLN:HB3	1:E:108:LEU:HD11	1.06	1.06
1:E:108:LEU:HD13	1:E:142:MET:SD	1.95	1.06
1:E:158:ARG:HB3	1:E:168:THR:HG21	1.46	0.97
1:C:51:LYS:H	1:C:51:LYS:HE3	1.31	0.96
1:E:42:ALA:HB2	1:E:69:VAL:HG11	1.52	0.90
1:D:100:LEU:O	1:D:101:THR:HG23	1.73	0.88
1:E:95:GLN:CB	1:E:108:LEU:HD11	1.99	0.88
1:E:57:PHE:HD2	1:E:125:LEU:HD22	1.38	0.88
1:E:57:PHE:CE2	1:E:139:MET:HB3	2.07	0.87
1:A:19:GLU:HG2	1:A:25:ARG:HG2	1.58	0.85
1:E:57:PHE:HZ	1:E:142:MET:CE	1.90	0.84
1:C:51:LYS:H	1:C:51:LYS:CE	1.90	0.83
1:C:51:LYS:N	1:C:51:LYS:HE3	1.94	0.83
1:E:3:THR:HG21	1:E:14:HIS:HB3	1.61	0.82
1:E:46:ARG:HB3	1:E:47:PRO:HD3	1.60	0.82
1:E:57:PHE:CD2	1:E:125:LEU:HD22	2.14	0.82
1:E:108:LEU:HD12	1:E:108:LEU:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ARG:HA	1:E:89:MET:HE1	1.66	0.78
1:E:95:GLN:HB3	1:E:108:LEU:CD1	2.02	0.77
1:E:157:PHE:HB3	1:E:172:LEU:HG	1.68	0.75
1:A:86:ARG:HH11	1:A:86:ARG:HG3	1.54	0.72
1:A:157:PHE:HB3	1:A:172:LEU:HG	1.72	0.71
1:E:30:GLU:HB2	5:E:1012:HOH:O	1.90	0.71
1:E:66:LEU:O	1:E:69:VAL:HG12	1.90	0.71
1:B:136:MET:HG2	1:B:139:MET:HE3	1.74	0.70
1:E:86:ARG:H	1:E:89:MET:HE2	1.58	0.69
1:A:86:ARG:HD3	5:A:2045:HOH:O	1.93	0.68
1:E:93:ILE:HD12	1:E:110:LEU:HD23	1.76	0.67
1:E:158:ARG:HD2	1:E:168:THR:OG1	1.94	0.67
1:E:164:LEU:HD13	1:E:166:VAL:HG23	1.75	0.67
1:E:63:PRO:HG3	1:E:128:ASP:HB2	1.75	0.67
1:A:51:LYS:H	1:A:51:LYS:CD	2.09	0.66
1:E:155:ALA:O	1:E:168:THR:HA	1.95	0.66
1:E:50:PRO:O	1:E:52:GLU:N	2.29	0.66
1:E:64:ILE:HD11	1:E:80:VAL:HG11	1.78	0.65
1:E:169:VAL:HG23	1:E:170:ALA:H	1.61	0.65
1:E:42:ALA:CB	1:E:69:VAL:HG11	2.25	0.65
1:C:129:VAL:HG22	1:C:157:PHE:HB2	1.77	0.65
1:A:18:ILE:HD13	1:A:28:LEU:HD13	1.79	0.64
1:C:158:ARG:HB2	1:C:168:THR:HG21	1.80	0.64
1:E:72:GLU:O	1:E:72:GLU:HG2	1.97	0.64
1:E:171:GLU:HG3	1:E:172:LEU:N	2.13	0.63
1:E:158:ARG:NE	1:E:171:GLU:OE1	2.31	0.63
1:A:51:LYS:H	1:A:51:LYS:CE	2.11	0.62
1:E:35:PRO:O	1:E:39:ARG:N	2.19	0.62
1:E:39:ARG:O	1:E:42:ALA:HB3	1.98	0.62
1:C:112:ARG:O	1:C:116:GLU:HG3	1.99	0.61
1:E:15:VAL:CG1	1:E:28:LEU:H	2.13	0.61
1:E:15:VAL:HG11	1:E:28:LEU:N	2.15	0.61
1:D:105:GLY:HA2	5:D:2037:HOH:O	2.01	0.61
1:E:57:PHE:HZ	1:E:142:MET:HE3	1.65	0.61
1:C:90:GLU:HB3	1:C:112:ARG:HB3	1.83	0.60
1:A:51:LYS:H	1:A:51:LYS:HD2	1.66	0.60
1:A:112:ARG:O	1:A:116:GLU:HG3	2.02	0.60
1:A:19:GLU:HG2	1:A:25:ARG:CG	2.32	0.60
1:E:57:PHE:HB2	1:E:123:VAL:CG1	2.32	0.60
1:E:39:ARG:O	1:E:43:GLU:HG3	2.02	0.60
1:D:99:THR:OG1	1:D:100:LEU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:MET:HA	1:E:139:MET:HE2	1.84	0.60
1:E:3:THR:CG2	1:E:4:TYR:N	2.64	0.59
1:A:29:VAL:HG21	1:A:129:VAL:CG2	2.32	0.59
1:E:66:LEU:HD21	1:E:156:VAL:HG23	1.84	0.59
1:E:15:VAL:HG13	1:E:28:LEU:O	2.03	0.59
1:E:55:ILE:HG23	1:E:123:VAL:HG13	1.85	0.58
1:E:3:THR:HG21	1:E:14:HIS:CB	2.31	0.58
1:C:4:TYR:CE2	1:C:173:PRO:HG3	2.38	0.58
1:E:48:LEU:HB3	1:E:154:LEU:HD22	1.85	0.58
1:E:158:ARG:CZ	1:E:171:GLU:HB2	2.34	0.58
1:E:49:VAL:O	1:E:51:LYS:N	2.34	0.58
1:E:169:VAL:HG23	1:E:170:ALA:N	2.19	0.57
1:E:54:GLU:O	1:E:77:PRO:HD2	2.04	0.57
1:E:26:ILE:HD12	1:E:159:GLN:HE22	1.69	0.57
1:C:18:ILE:HD13	1:C:28:LEU:HD13	1.87	0.57
1:E:108:LEU:CD1	1:E:142:MET:SD	2.84	0.56
1:E:123:VAL:O	1:E:150:VAL:HA	2.05	0.56
1:B:4:TYR:HB2	1:B:17:LEU:HD21	1.88	0.56
1:A:21:LEU:HB3	1:A:22:PRO:HD2	1.88	0.56
1:E:135:THR:O	1:E:139:MET:HG3	2.06	0.56
1:E:3:THR:HG22	1:E:4:TYR:N	2.21	0.55
1:E:57:PHE:CZ	1:E:142:MET:CE	2.81	0.55
1:E:57:PHE:CZ	1:E:142:MET:HE3	2.41	0.55
1:A:127:SER:O	1:A:155:ALA:HA	2.07	0.55
1:E:15:VAL:HG12	1:E:16:PRO:O	2.07	0.55
1:E:57:PHE:HE2	1:E:139:MET:CB	2.04	0.55
1:E:86:ARG:H	1:E:89:MET:CE	2.19	0.55
1:A:19:GLU:CG	1:A:25:ARG:HG2	2.33	0.55
1:E:56:LEU:HD23	1:E:124:VAL:HB	1.88	0.55
1:E:68:HIS:HD2	1:E:78:TYR:OH	1.90	0.55
1:E:69:VAL:CG1	1:E:70:LEU:N	2.69	0.55
1:E:85:ARG:O	1:E:85:ARG:HG3	2.06	0.55
1:C:29:VAL:HG11	1:C:129:VAL:HG23	1.89	0.54
1:E:111:ASP:OD2	1:E:113:ARG:HB2	2.06	0.54
1:E:26:ILE:CD1	1:E:159:GLN:HE22	2.20	0.54
1:D:18:ILE:HD13	1:D:28:LEU:HD13	1.89	0.54
1:E:137:ARG:NH2	1:E:164:LEU:HB3	2.23	0.54
1:E:57:PHE:O	1:E:125:LEU:HA	2.08	0.54
1:E:42:ALA:HB2	1:E:69:VAL:CG1	2.29	0.53
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.72	0.53
1:A:20:PRO:HG2	1:A:26:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:VAL:HG12	1:E:130:VAL:N	2.24	0.53
1:E:69:VAL:HG13	1:E:70:LEU:N	2.23	0.53
1:E:15:VAL:CG1	1:E:28:LEU:N	2.72	0.53
1:A:51:LYS:N	1:A:51:LYS:HD2	2.24	0.53
1:B:127:SER:O	1:B:155:ALA:HA	2.09	0.53
1:C:90:GLU:O	1:C:91:ASP:C	2.47	0.53
1:D:158:ARG:HG2	1:D:160:GLY:O	2.09	0.53
1:E:46:ARG:HB3	1:E:47:PRO:CD	2.36	0.53
1:E:42:ALA:CB	1:E:69:VAL:CG1	2.86	0.53
1:C:46:ARG:HB2	1:C:47:PRO:HD3	1.91	0.52
1:E:155:ALA:HB3	1:E:168:THR:HG22	1.90	0.52
1:C:86:ARG:O	1:C:89:MET:HB2	2.10	0.52
1:D:4:TYR:CE2	1:D:175:LEU:HD21	2.44	0.52
1:E:136:MET:HG2	5:E:1007:HOH:O	2.10	0.51
1:E:57:PHE:HB2	1:E:123:VAL:HG11	1.92	0.51
1:E:46:ARG:O	1:E:48:LEU:N	2.43	0.51
1:A:171:GLU:HG3	1:A:172:LEU:N	2.24	0.51
1:E:158:ARG:NE	1:E:171:GLU:HB2	2.25	0.51
1:E:64:ILE:N	1:E:65:PRO:HD2	2.26	0.51
1:E:8:VAL:C	1:E:10:GLY:H	2.13	0.51
1:C:90:GLU:O	1:C:92:PRO:N	2.43	0.51
1:A:98:GLN:HB2	1:A:134:GLU:OE1	2.10	0.51
1:A:140:GLU:O	1:A:144:LEU:HG	2.11	0.51
1:E:86:ARG:N	1:E:89:MET:HE2	2.26	0.51
1:A:90:GLU:O	1:A:91:ASP:C	2.48	0.51
1:E:91:ASP:O	1:E:112:ARG:HB2	2.10	0.50
1:C:6:ILE:HD11	1:C:15:VAL:HG11	1.92	0.50
1:E:125:LEU:HG	1:E:150:VAL:HG11	1.93	0.50
1:E:5:PRO:HG3	1:E:14:HIS:NE2	2.27	0.50
1:B:59:THR:HG23	1:B:139:MET:SD	2.52	0.49
1:A:144:LEU:HB3	5:D:2042:HOH:O	2.12	0.49
1:C:155:ALA:O	1:C:168:THR:HA	2.12	0.49
1:E:31:PHE:HE2	1:E:66:LEU:HD22	1.77	0.49
1:A:95:GLN:HG3	1:A:142:MET:CG	2.43	0.49
1:D:7:THR:HG22	1:D:12:THR:OG1	2.12	0.49
1:E:8:VAL:O	1:E:10:GLY:N	2.42	0.49
1:E:46:ARG:C	1:E:48:LEU:H	2.15	0.49
1:E:7:THR:HG22	1:E:12:THR:HA	1.95	0.49
1:C:83:ARG:HB3	1:D:84:ARG:HH22	1.78	0.49
1:A:46:ARG:HG3	1:A:74:LEU:HD21	1.95	0.48
1:E:131:ALA:O	1:E:162:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PHE:HD1	1:D:58:THR:N	2.10	0.48
1:E:48:LEU:CB	1:E:154:LEU:HD22	2.43	0.48
1:D:90:GLU:O	1:D:91:ASP:C	2.51	0.48
1:A:51:LYS:H	1:A:51:LYS:HE3	1.77	0.48
1:A:86:ARG:CG	1:A:86:ARG:HH11	2.25	0.47
1:B:112:ARG:O	1:B:116:GLU:HG3	2.14	0.47
1:A:95:GLN:HG3	1:A:142:MET:HG2	1.95	0.47
1:D:137:ARG:HD3	5:D:2080:HOH:O	2.14	0.47
1:E:62:SER:O	1:E:65:PRO:HG2	2.14	0.47
1:A:149:HIS:CD2	1:C:43:GLU:HG3	2.49	0.47
1:D:131:ALA:O	1:D:162:PRO:HA	2.14	0.47
1:E:95:GLN:O	1:E:108:LEU:HG	2.14	0.47
1:E:30:GLU:O	1:E:30:GLU:HG3	2.15	0.47
1:D:119:LEU:HG	1:D:120:ASN:ND2	2.30	0.47
1:C:59:THR:HG22	1:C:81:ALA:HB3	1.95	0.47
1:E:49:VAL:HB	1:E:51:LYS:HE3	1.96	0.46
1:B:86:ARG:NH2	3:B:1001:CL:CL	2.84	0.46
1:E:29:VAL:HG21	1:E:157:PHE:CD1	2.50	0.46
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.81	0.46
1:D:99:THR:HB	1:D:105:GLY:CA	2.46	0.46
1:C:29:VAL:HG11	1:C:129:VAL:CG2	2.46	0.46
1:C:158:ARG:CZ	1:C:162:PRO:HG2	2.46	0.46
1:E:93:ILE:HD11	1:E:115:ALA:HB1	1.98	0.46
1:A:162:PRO:C	1:A:164:LEU:H	2.20	0.45
1:E:15:VAL:HG12	1:E:28:LEU:H	1.82	0.45
1:C:129:VAL:HG12	1:C:130:VAL:N	2.32	0.45
1:E:125:LEU:HD13	1:E:139:MET:HE3	1.98	0.45
1:C:4:TYR:CD1	1:C:175:LEU:HD11	2.52	0.45
1:E:49:VAL:HB	1:E:51:LYS:HD2	1.98	0.45
1:B:131:ALA:O	1:B:162:PRO:HA	2.16	0.44
1:C:158:ARG:NH1	1:C:162:PRO:HD2	2.32	0.44
1:E:56:LEU:CD2	1:E:124:VAL:HB	2.47	0.44
1:A:29:VAL:HG23	1:A:29:VAL:O	2.16	0.44
1:B:49:VAL:HG21	1:B:74:LEU:HD11	1.98	0.44
1:E:90:GLU:O	1:E:91:ASP:C	2.55	0.44
1:A:15:VAL:HG12	5:A:2054:HOH:O	2.17	0.44
1:D:64:ILE:HB	1:D:65:PRO:HD3	1.99	0.44
1:C:136:MET:HG3	5:C:2033:HOH:O	2.17	0.44
1:A:51:LYS:N	1:A:51:LYS:CD	2.76	0.44
1:C:78:TYR:CE1	1:D:33:GLY:HA2	2.52	0.44
1:E:64:ILE:CD1	1:E:80:VAL:HG11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:HA	1:E:61:THR:HA	1.67	0.43
1:E:66:LEU:HD21	1:E:156:VAL:CG2	2.48	0.43
1:A:72:GLU:HB2	1:B:35:PRO:HB3	2.01	0.43
1:A:158:ARG:HB3	1:A:158:ARG:HE	1.63	0.43
1:E:136:MET:CE	1:E:153:ARG:HB3	2.49	0.43
1:E:158:ARG:HG2	1:E:158:ARG:O	2.17	0.43
1:B:136:MET:HA	1:B:139:MET:HE2	2.00	0.43
1:A:84:ARG:NH1	1:B:84:ARG:NE	2.67	0.43
1:D:99:THR:HB	1:D:105:GLY:HA3	1.99	0.43
1:D:127:SER:O	1:D:155:ALA:HA	2.17	0.43
1:D:79:VAL:HG12	1:D:114:PHE:CD1	2.53	0.43
1:D:99:THR:HG23	1:D:100:LEU:N	2.34	0.43
1:B:4:TYR:CE2	1:B:173:PRO:HG3	2.54	0.42
1:B:71:ALA:HB1	1:B:76:LEU:O	2.18	0.42
1:B:50:PRO:HG2	1:B:152:ALA:HB2	2.00	0.42
1:E:46:ARG:C	1:E:48:LEU:N	2.73	0.42
1:C:84:ARG:HB3	1:D:84:ARG:NH1	2.34	0.42
1:A:55:ILE:HD13	1:A:118:LEU:HD23	2.01	0.42
1:A:18:ILE:O	1:A:20:PRO:HD3	2.19	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.27	0.42
1:A:46:ARG:N	1:A:47:PRO:HD2	2.34	0.42
1:B:113:ARG:HG3	5:B:2066:HOH:O	2.19	0.42
1:A:149:HIS:CG	1:C:43:GLU:HG3	2.55	0.41
1:D:82:ARG:NH2	1:D:86:ARG:NH1	2.68	0.41
1:D:85:ARG:HD2	5:D:2084:HOH:O	2.21	0.41
1:E:35:PRO:O	1:E:36:GLU:C	2.59	0.41
1:E:49:VAL:HB	1:E:51:LYS:CE	2.51	0.41
1:A:32:LEU:HG	1:A:62:SER:HA	2.01	0.41
1:C:33:GLY:HA2	1:D:78:TYR:CE1	2.56	0.41
1:B:154:LEU:HD23	1:B:167:ASP:HB2	2.01	0.41
1:E:110:LEU:HD23	1:E:115:ALA:HB2	2.03	0.41
1:E:7:THR:HG22	1:E:12:THR:OG1	2.21	0.41
1:A:57:PHE:HD1	1:A:58:THR:N	2.19	0.41
1:D:4:TYR:HE2	1:D:175:LEU:HD21	1.86	0.41
1:B:155:ALA:O	1:B:168:THR:HA	2.21	0.41
1:C:33:GLY:HA2	1:D:78:TYR:CD1	2.56	0.40
1:A:6:ILE:HD13	1:A:29:VAL:HG12	2.02	0.40
1:B:46:ARG:NH1	1:B:46:ARG:HG2	2.36	0.40
1:C:158:ARG:NE	1:C:162:PRO:HG2	2.36	0.40
1:B:96:GLU:HG3	5:B:2061:HOH:O	2.21	0.40
1:E:59:THR:CG2	1:E:60:GLU:N	2.83	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	165/175 (94%)	162 (98%)	3 (2%)	0	100	100
1	B	166/175 (95%)	161 (97%)	4 (2%)	1 (1%)	25	13
1	C	166/175 (95%)	164 (99%)	1 (1%)	1 (1%)	25	13
1	D	169/175 (97%)	165 (98%)	3 (2%)	1 (1%)	25	13
1	E	136/175 (78%)	120 (88%)	12 (9%)	4 (3%)	4	0
All	All	802/875 (92%)	772 (96%)	23 (3%)	7 (1%)	17	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	51	LYS
1	E	47	PRO
1	C	91	ASP
1	B	91	ASP
1	E	91	ASP
1	E	9	GLY
1	D	91	ASP

### 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	142/147 (97%)	139 (98%)	3 (2%)	53	41
1	B	143/147 (97%)	141 (99%)	2 (1%)	67	58
1	C	142/147 (97%)	141 (99%)	1 (1%)	84	81
1	D	146/147 (99%)	145 (99%)	1 (1%)	84	81
1	E	126/147 (86%)	121 (96%)	5 (4%)	31	16
All	All	699/735 (95%)	687 (98%)	12 (2%)	60	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	57	PHE
1	A	171	GLU
1	B	57	PHE
1	B	122	ARG
1	C	51	LYS
1	D	57	PHE
1	E	84	ARG
1	E	128	ASP
1	E	158	ARG
1	E	159	GLN
1	E	164	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	98	GLN
1	A	149	HIS
1	B	159	GLN
1	C	120	ASN
1	C	159	GLN
1	D	98	GLN
1	D	120	ASN
1	D	159	GLN
1	E	68	HIS
1	E	159	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z  > 2$
2	ACY	C	2003	-	1,3,3	2.27	1 (100%)	0,3,3	0.00	-
2	ACY	A	2002	-	1,3,3	2.49	1 (100%)	0,3,3	0.00	-
2	ACY	B	2001	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-
2	ACY	D	2004	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ACY	CH3-C	2.51	1.51	1.48
2	A	2002	ACY	CH3-C	2.49	1.51	1.48
2	D	2004	ACY	CH3-C	2.45	1.51	1.48
2	C	2003	ACY	CH3-C	2.27	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	169/175 (96%)	0.32	8 (4%) 31 39	18, 39, 73, 85	0
1	B	170/175 (97%)	0.08	2 (1%) 79 83	20, 37, 57, 77	0
1	C	170/175 (97%)	0.18	6 (3%) 44 51	21, 40, 70, 96	0
1	D	173/175 (98%)	0.33	6 (3%) 44 51	22, 36, 63, 95	0
1	E	152/175 (86%)	2.33	76 (50%) 0 0	44, 74, 91, 99	0
All	All	834/875 (95%)	0.61	98 (11%) 4 7	18, 41, 83, 99	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	123	VAL	10.0
1	E	124	VAL	9.2
1	E	108	LEU	8.6
1	A	99	THR	6.8
1	E	66	LEU	6.8
1	D	100	LEU	6.5
1	E	69	VAL	6.5
1	E	162	PRO	6.2
1	E	154	LEU	5.5
1	E	156	VAL	5.4
1	E	143	VAL	5.3
1	E	118	LEU	5.2
1	D	101	THR	5.1
1	A	163	GLY	5.0
1	E	93	ILE	5.0
1	E	79	VAL	4.8
1	E	52	GLU	4.8
1	E	114	PHE	4.7
1	C	175	LEU	4.6
1	E	169	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	53	ALA	4.5
1	E	170	ALA	4.4
1	D	104	VAL	4.3
1	E	56	LEU	4.2
1	E	126	VAL	4.2
1	E	48	LEU	4.1
1	E	110	LEU	4.0
1	E	161	THR	4.0
1	E	31	PHE	4.0
1	E	144	LEU	4.0
1	E	55	ILE	3.9
1	E	68	HIS	3.8
1	E	163	GLY	3.8
1	E	139	MET	3.8
1	E	136	MET	3.8
1	E	54	GLU	3.7
1	E	47	PRO	3.7
1	E	130	VAL	3.7
1	E	105	GLY	3.5
1	E	121	GLN	3.5
1	E	142	MET	3.5
1	E	50	PRO	3.5
1	E	132	SER	3.4
1	E	43	GLU	3.4
1	E	167	ASP	3.3
1	D	105	GLY	3.3
1	D	99	THR	3.2
1	E	116	GLU	3.1
1	A	162	PRO	3.1
1	C	162	PRO	3.0
1	E	149	HIS	2.9
1	C	98	GLN	2.9
1	E	145	ARG	2.9
1	E	2	GLU	2.9
1	E	92	PRO	2.9
1	E	111	ASP	2.9
1	E	109	TRP	2.8
1	A	98	GLN	2.8
1	E	107	VAL	2.8
1	D	98	GLN	2.8
1	E	106	GLU	2.8
1	E	85	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	99	THR	2.7
1	E	122	ARG	2.7
1	E	96	GLU	2.7
1	C	1	MET	2.7
1	A	175	LEU	2.7
1	E	7	THR	2.7
1	E	71	ALA	2.6
1	E	171	GLU	2.6
1	E	57	PHE	2.6
1	E	49	VAL	2.6
1	E	15	VAL	2.5
1	E	35	PRO	2.5
1	E	14	HIS	2.5
1	A	161	THR	2.4
1	E	46	ARG	2.4
1	E	95	GLN	2.4
1	E	150	VAL	2.4
1	E	138	ALA	2.3
1	A	97	VAL	2.3
1	B	175	LEU	2.3
1	E	125	LEU	2.3
1	E	129	VAL	2.3
1	E	78	TYR	2.2
1	A	4	TYR	2.2
1	E	30	GLU	2.2
1	E	157	PHE	2.2
1	E	16	PRO	2.1
1	E	137	ARG	2.1
1	E	64	ILE	2.1
1	E	8	VAL	2.1
1	C	164	LEU	2.1
1	E	29	VAL	2.1
1	E	45	LEU	2.1
1	E	51	LYS	2.1
1	C	174	VAL	2.0
1	E	172	LEU	2.0

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

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	E	1005	1/1	0.78	0.26	84,84,84,84	0
2	ACY	A	2002	4/4	0.89	0.18	59,60,60,66	0
3	CL	B	1001	1/1	0.91	0.21	68,68,68,68	0
3	CL	B	1002	1/1	0.93	0.17	56,56,56,56	0
2	ACY	D	2004	4/4	0.95	0.09	35,40,41,44	0
2	ACY	B	2001	4/4	0.95	0.10	37,40,40,45	0
2	ACY	C	2003	4/4	0.96	0.14	64,65,69,70	0
3	CL	C	1003	1/1	0.97	0.33	59,59,59,59	0
4	CA	C	1006	1/1	0.98	0.06	36,36,36,36	0
3	CL	D	1004	1/1	0.98	0.26	50,50,50,50	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.