



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2016 – 11:45 PM EDT

PDB ID : 5B5T  
Title : Crystal Structure of Escherichia coli Gamma-Glutamyltranspeptidase in Complex with peptidyl phosphonate inhibitor 1b  
Authors : Wada, K.; Fukuyama, K.  
Deposited on : 2016-05-18  
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

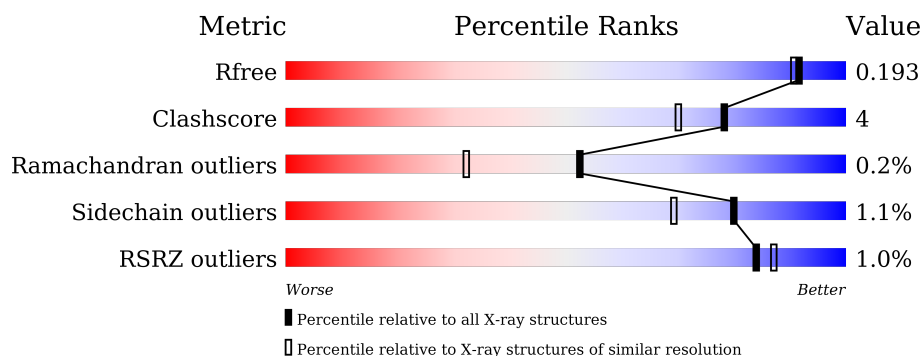
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	366	<div> <div>86%</div> <div>9% 5%</div> </div>
1	C	366	<div> <div>2%</div> <div>90%</div> <div>5% 5%</div> </div>
2	B	190	<div> <div>2%</div> <div>89%</div> <div>11% .</div> </div>
2	D	190	<div> <div>2%</div> <div>91%</div> <div>9% .</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9416 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.

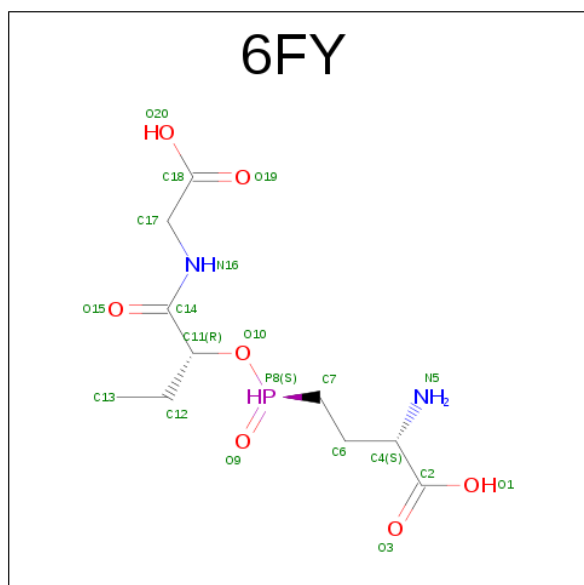
- Molecule 1 is a protein called Gamma-glutamyltranspeptidase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2643	1670	446	516	11			
1	C	349	Total	C	N	O	S	0	0	0
			2643	1670	446	516	11			

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1407	882	238	282	5			
2	D	190	Total	C	N	O	S	0	0	0
			1407	882	238	282	5			

- Molecule 3 is (2 {S})-2-azanyl-4-[(2 {R})-1-(2-hydroxy-2-oxoethylamino)-1-oxidanylidene-butan-2-yl]oxyphosphonoyl-butanoic acid (three-letter code: 6FY) (formula: C<sub>10</sub>H<sub>19</sub>N<sub>2</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
3	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	467	Total	O	0	0
			467	467		
5	B	190	Total	O	0	0
			190	190		
5	C	425	Total	O	0	0
			425	425		
5	D	192	Total	O	0	0
			192	192		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.99 Å 126.39 Å 129.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.33 – 1.70 46.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (37.33-1.70) 95.8 (46.27-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.70 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.178 , 0.194 0.176 , 0.193	Depositor DCC
$R_{free}$ test set	6667 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 6FY

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	0.36	0/2696	0.56	1/3648 (0.0%)
1	C	0.35	0/2696	0.53	0/3648
2	B	0.37	0/1434	0.58	0/1952
2	D	0.36	0/1434	0.59	0/1952
All	All	0.36	0/8260	0.56	1/11200 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	MET	CG-SD-CE	5.30	108.68	100.20

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	2643	0	2614	29	0
1	C	2643	0	2614	15	0
2	B	1407	0	1391	14	0
2	D	1407	0	1391	10	0
3	B	20	0	0	2	0
3	D	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	467	0	0	2	1
5	B	190	0	0	2	0
5	C	425	0	0	2	0
5	D	192	0	0	1	1
All	All	9416	0	8010	58	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 4.

All (58) 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:A:290:MET:HE3	1:A:291:PRO:HD2	1.61	0.83
1:A:373:LYS:HD2	1:A:378:ILE:HD11	1.64	0.78
1:A:164:MET:HE3	1:A:168:LYS:HG2	1.64	0.77
1:C:200:PRO:O	1:C:206:LYS:NZ	2.19	0.75
2:D:391:THR:HG23	2:D:409:THR:HB	1.69	0.74
2:B:391:THR:HG23	2:B:409:THR:HB	1.70	0.74
2:D:548:GLU:OE1	2:D:549:ALA:N	2.22	0.69
1:C:313:LYS:HD2	2:D:500:ASP:O	1.93	0.69
1:A:164:MET:HE3	1:A:168:LYS:HE3	1.73	0.68
1:A:257:LYS:HE2	1:A:257:LYS:HA	1.80	0.64
1:C:103:SER:OG	1:C:105:ASN:OD1	2.17	0.62
1:A:45:ARG:CZ	1:A:45:ARG:HB3	2.30	0.60
1:A:164:MET:HE3	1:A:168:LYS:CG	2.32	0.59
1:A:369:ILE:O	2:B:540:LYS:HE3	2.03	0.58
2:B:474:LYS:NZ	5:B:701:HOH:O	2.38	0.57
1:C:89:GLN:HB2	2:D:413:THR:HG23	1.88	0.55
1:A:164:MET:CE	1:A:168:LYS:HE3	2.36	0.55
2:D:411:ASN:HB3	2:D:429:ASN:OD1	2.06	0.55
2:B:411:ASN:HB3	2:B:429:ASN:OD1	2.08	0.53
1:A:249:GLU:O	1:A:253:GLN:HG3	2.08	0.53
1:A:332:TYR:CE1	1:A:378:ILE:HD12	2.45	0.52
1:A:317:PHE:CZ	2:B:511:ALA:HB1	2.46	0.51
1:C:171:GLN:OE1	1:C:175:LYS:HE3	2.11	0.50
2:B:482:PRO:HG2	3:B:600:6FY:O19	2.12	0.50
1:A:111:ILE:HD12	1:A:156:LEU:HD22	1.93	0.50
1:C:249:GLU:OE1	1:C:264:LYS:HD2	2.11	0.50
2:B:505:VAL:HB	2:B:557:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HB3	1:C:45:ARG:HH11	1.76	0.49
2:D:563:GLU:HG2	2:D:565:TYR:CE2	2.48	0.48
1:A:107:ASN:HB2	5:A:731:HOH:O	2.14	0.48
1:A:298:ILE:HG12	5:A:459:HOH:O	2.13	0.48
1:C:317:PHE:CZ	2:D:511:ALA:HB1	2.49	0.48
2:D:566:GLY:HA3	2:D:577:THR:HG21	1.97	0.46
1:C:217:LYS:HD2	5:C:500:HOH:O	2.16	0.46
1:C:289:SER:HB3	1:C:297:GLY:HA2	1.96	0.46
1:A:120:LYS:HD3	1:A:120:LYS:HA	1.63	0.44
1:A:68:GLU:OE2	1:A:168:LYS:NZ	2.31	0.44
1:C:255:MET:HG3	1:C:262:ILE:HB	1.99	0.43
1:A:334:TYR:CD2	2:B:517:GLN:HA	2.53	0.43
1:A:202:HIS:CE1	2:B:418:ILE:HG12	2.53	0.43
1:C:210:TRP:CH2	1:C:215:PRO:HB3	2.54	0.43
1:A:229:LYS:HA	1:A:229:LYS:HD3	1.87	0.42
1:A:229:LYS:HD2	1:A:233:MET:HG2	2.01	0.42
2:D:570:PRO:HA	5:D:840:HOH:O	2.19	0.42
2:B:517:GLN:O	2:B:518:TRP:HB3	2.19	0.42
2:B:566:GLY:HA3	2:B:577:THR:HG21	2.01	0.42
1:A:289:SER:HB3	1:A:297:GLY:HA2	2.01	0.41
1:A:99:MET:HG3	2:B:406:VAL:HG22	2.02	0.41
1:C:296:GLY:HA3	2:D:465:SER:OG	2.20	0.41
1:A:164:MET:CE	1:A:168:LYS:HG2	2.43	0.41
1:A:233:MET:HB3	1:A:241:GLU:HG2	2.02	0.41
1:A:249:GLU:OE2	1:A:264:LYS:HD2	2.19	0.41
1:A:56:ALA:O	1:A:60:GLN:HG3	2.21	0.41
2:B:570:PRO:HA	5:B:843:HOH:O	2.21	0.41
2:B:433:ASP:OD2	3:B:600:6FY:N5	2.54	0.40
1:C:171:GLN:HB3	1:C:172:PRO:HD3	2.02	0.40
1:A:255:MET:HG3	1:A:262:ILE:HB	2.03	0.40
1:C:105:ASN:ND2	5:C:423:HOH:O	2.55	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)
5:A:559:HOH:O	5:D:866:HOH:O[2_555]	2.19	0.01

## 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	347/366 (95%)	341 (98%)	6 (2%)	0	100	100
1	C	347/366 (95%)	341 (98%)	6 (2%)	0	100	100
2	B	188/190 (99%)	180 (96%)	7 (4%)	1 (0%)	34	15
2	D	188/190 (99%)	181 (96%)	6 (3%)	1 (0%)	34	15
All	All	1070/1112 (96%)	1043 (98%)	25 (2%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN
2	D	411	ASN

### 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	274/287 (96%)	272 (99%)	2 (1%)	88	82
1	C	274/287 (96%)	273 (100%)	1 (0%)	93	90
2	B	154/154 (100%)	151 (98%)	3 (2%)	65	46
2	D	154/154 (100%)	151 (98%)	3 (2%)	65	46
All	All	856/882 (97%)	847 (99%)	9 (1%)	80	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	210	TRP
2	B	408	TYR
2	B	486	ARG
2	B	523	LEU
1	C	210	TRP
2	D	408	TYR
2	D	486	ARG
2	D	535	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	6FY	B	600	2	9,19,19	0.86	0	6,24,24	4.05	3 (50%)
3	6FY	D	600	2	9,19,19	1.23	2 (22%)	6,24,24	2.53	2 (33%)

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	6FY	B	600	2	-	1/12/24/24	0/0/0/0
3	6FY	D	600	2	-	1/12/24/24	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	600	6FY	C17-N16	2.14	1.50	1.46
3	D	600	6FY	C14-N16	2.62	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	6FY	P8-C7-C6	-2.08	106.60	112.07
3	D	600	6FY	C11-C14-N16	2.21	120.63	116.63
3	B	600	6FY	C11-C14-N16	3.74	123.39	116.63
3	D	600	6FY	C17-N16-C14	5.20	129.71	122.36
3	B	600	6FY	C17-N16-C14	8.55	134.45	122.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	600	6FY	C11-C14-N16-C17
3	B	600	6FY	C11-C14-N16-C17

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	6FY	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	349/366 (95%)	-0.25	1 (0%) 94 95	15, 22, 33, 46	0
1	C	349/366 (95%)	-0.04	4 (1%) 82 86	13, 22, 37, 51	0
2	B	190/190 (100%)	-0.07	3 (1%) 74 79	15, 19, 34, 49	0
2	D	190/190 (100%)	0.08	3 (1%) 74 79	13, 20, 35, 50	0
All	All	1078/1112 (96%)	-0.09	11 (1%) 84 87	13, 21, 35, 51	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	560	PRO	6.4
2	D	561	ASP	4.5
1	C	387	GLU	3.0
2	B	561	ASP	2.8
1	C	315	TYR	2.4
2	B	560	PRO	2.3
2	D	535	LYS	2.3
1	A	387	GLU	2.3
1	C	384	ALA	2.2
2	B	535	LYS	2.2
1	C	212	GLU	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 ⓘ

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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	6FY	B	600	20/20	0.95	0.12	1.55	18,25,41,41	0
3	6FY	D	600	20/20	0.94	0.14	1.33	16,27,42,48	0
4	CA	D	601	1/1	0.99	0.06	-1.77	18,18,18,18	0
4	CA	B	601	1/1	0.99	0.03	-5.17	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.