



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:13 AM GMT

PDB ID : 2PUT  
Title : The crystal structure of isomerase domain of glucosamine-6-phosphate synthase from *Candida albicans*  
Authors : Raczynska, J.; Olchow, J.; Milewski, S.; Rypniewski, W.  
Deposited on : 2007-05-09  
Resolution : 1.90 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 (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

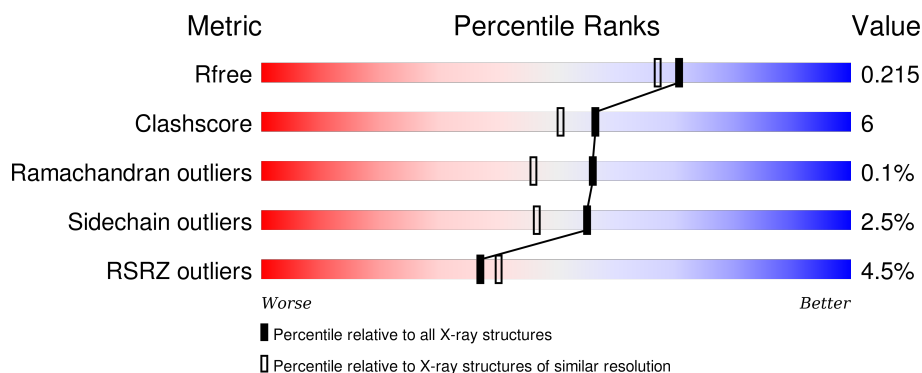
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	367	<div> <div>4%</div> <div>81% 11% • 8%</div> </div>
1	B	367	<div> <div>4%</div> <div>82% 13% • •</div> </div>
1	C	367	<div> <div>6%</div> <div>80% 14% • 5%</div> </div>
1	D	367	<div> <div>4%</div> <div>82% 10% • 7%</div> </div>

## 2 Entry composition [i](#)

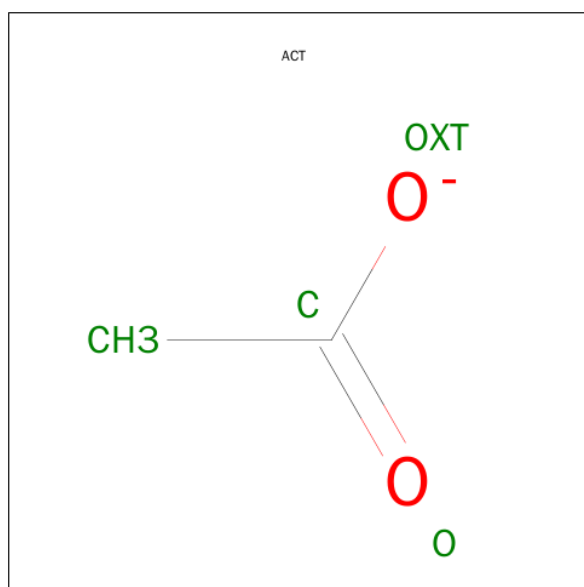
There are 6 unique types of molecules in this entry. The entry contains 11779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	2	0
			2642	1669	459	497	17			
1	B	352	Total	C	N	O	S	0	2	0
			2742	1730	476	519	17			
1	C	350	Total	C	N	O	S	0	6	0
			2745	1735	474	518	18			
1	D	341	Total	C	N	O	S	0	4	0
			2670	1685	462	506	17			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

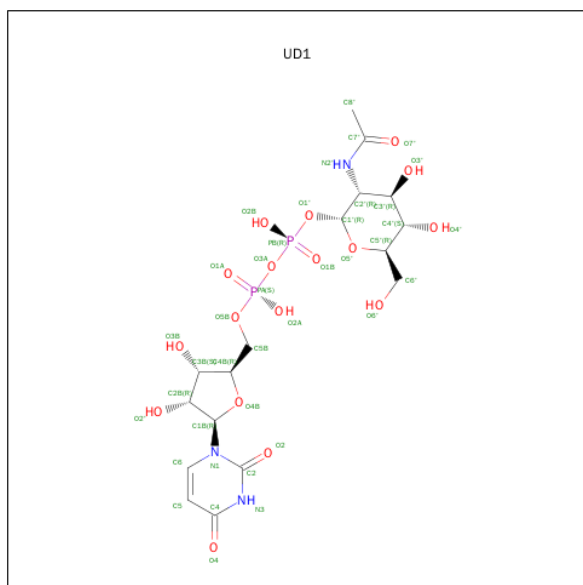


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

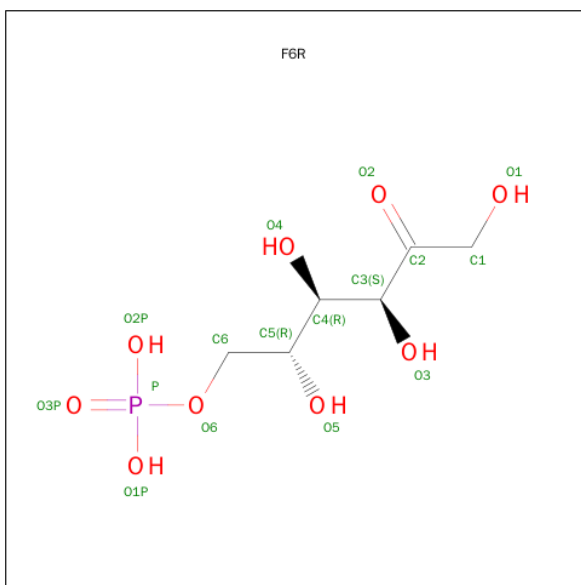
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
4	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 5 is FRUCTOSE -6-PHOSPHATE (three-letter code: F6R) (formula:  $C_6H_{13}O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			16	6	9	1		
5	B	1	Total	C	O	P	0	0
			16	6	9	1		
5	C	1	Total	C	O	P	0	0
			16	6	9	1		
5	D	1	Total	C	O	P	0	0
			16	6	9	1		

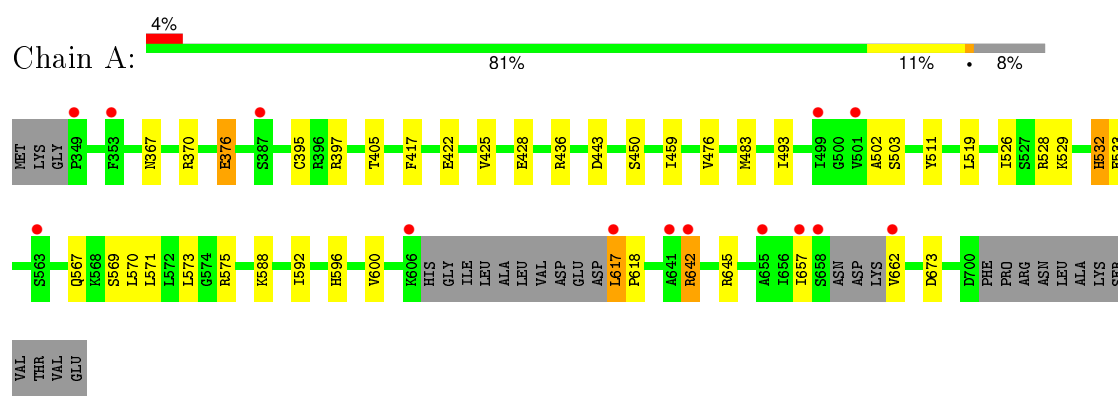
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	196	Total	O	0	0
			196	196		
6	B	189	Total	O	0	0
			189	189		
6	C	168	Total	O	0	0
			168	168		
6	D	195	Total	O	0	0
			195	195		

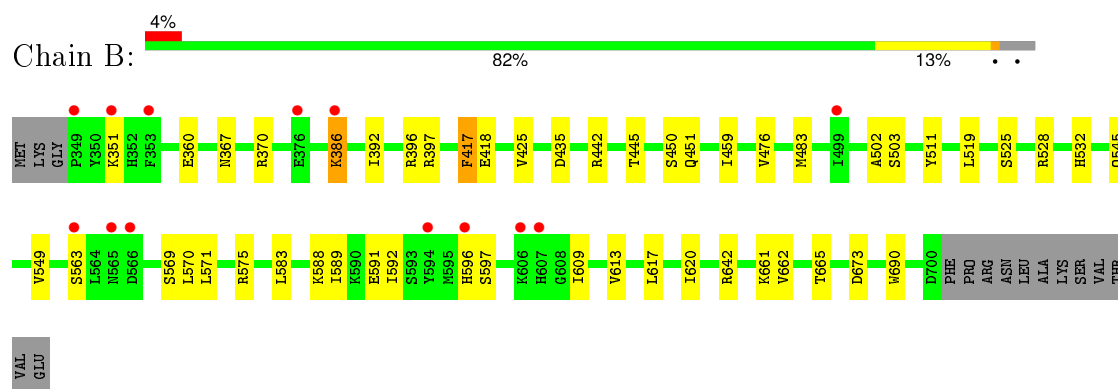
### 3 Residue-property plots [i](#)

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.

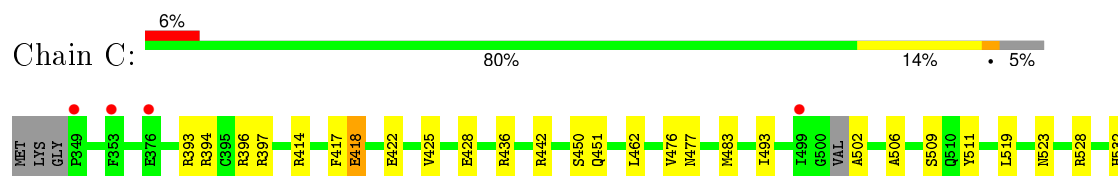
- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)

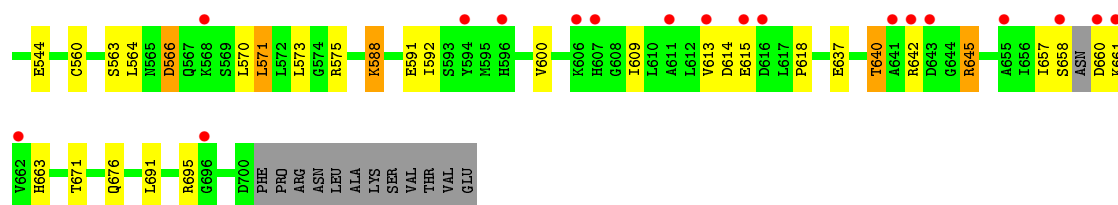


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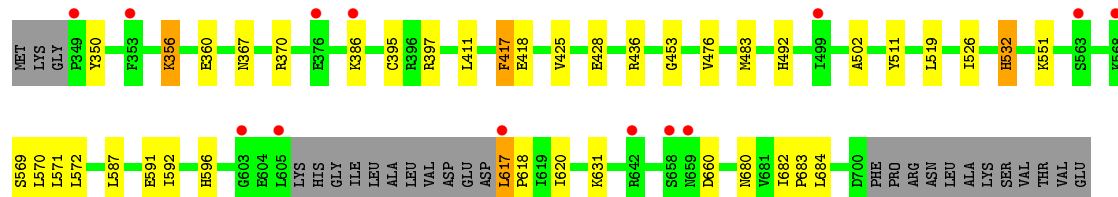
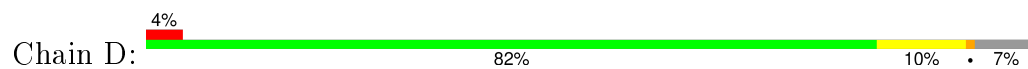


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- Molecule 1: isomerase domain of glutamine-fructose-6-phosphate transaminase (isomerizing)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.03Å 118.19Å 100.03Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 19.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.90) 99.7 (19.94-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.171 , 0.215 0.171 , 0.215	Depositor DCC
$R_{free}$ test set	2419 reflections (2.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.1	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 120111 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, UD1, F6R, ACT

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	0.82	0/2687	0.83	2/3627 (0.1%)
1	B	0.78	0/2790	0.81	4/3770 (0.1%)
1	C	0.79	2/2803 (0.1%)	0.78	1/3783 (0.0%)
1	D	0.81	0/2722	0.84	1/3676 (0.0%)
All	All	0.80	2/11002 (0.0%)	0.82	8/14856 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	418	GLU	CD-OE1	5.75	1.31	1.25
1	C	418	GLU	CG-CD	5.04	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	662	VAL	N-CA-C	-8.78	87.28	111.00
1	B	575	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	673	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	411	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	B	673	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	583	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	A	673	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	575	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	661	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2702	34	0
1	B	2742	0	2798	32	0
1	C	2745	0	2812	42	0
1	D	2670	0	2725	32	0
2	A	4	0	3	0	0
2	C	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	25	1	0
4	B	39	0	25	0	0
4	C	39	0	25	1	0
4	D	39	0	25	1	0
5	A	16	0	11	1	0
5	B	16	0	11	1	0
5	C	16	0	11	1	0
5	D	16	0	11	1	0
6	A	196	0	0	4	0
6	B	189	0	0	4	0
6	C	168	0	0	4	0
6	D	195	0	0	7	0
All	All	11779	0	11187	135	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 6.

All (135) 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:459:ILE:HD13	1:B:483:MET:SD	1.92	1.10
1:C:502:ALA:HB3	1:C:592:ILE:HD11	1.34	1.08
1:B:386:LYS:HA	6:B:5565:HOH:O	1.54	1.07
1:C:502:ALA:CB	1:C:592:ILE:HD11	1.87	1.04
1:A:493:ILE:HD11	6:A:5691:HOH:O	1.71	0.90
1:C:451[B]:GLN:HE22	1:C:493:ILE:HD11	1.36	0.88
1:A:642:ARG:HG3	1:A:642:ARG:O	1.71	0.87
1:B:351:LYS:HE3	1:B:690:TRP:HH2	1.40	0.85
1:B:502:ALA:HB2	1:B:592:ILE:HD11	1.59	0.83
1:A:567:GLN:HG3	1:A:618:PRO:HG3	1.63	0.79
1:C:451[B]:GLN:NE2	1:C:493:ILE:HD11	2.02	0.74
1:C:428:GLU:OE1	1:C:436[A]:ARG:NH2	2.20	0.73
1:A:395:CYS:HB3	1:C:442[B]:ARG:NH1	2.04	0.72
1:B:351:LYS:HE3	1:B:690:TRP:CH2	2.25	0.72
1:B:591:GLU:OE1	5:B:5004:F6R:H1C1	1.90	0.71
1:A:570:LEU:HD13	1:A:618:PRO:HB2	1.74	0.70
1:C:591:GLU:OE1	5:C:5005:F6R:H1C1	1.92	0.69
1:A:526:ILE:HD13	1:D:526:ILE:HG12	1.75	0.69
1:D:428:GLU:OE1	1:D:436[A]:ARG:NH2	2.25	0.68
1:D:350:TYR:HD2	1:D:356:LYS:HE3	1.58	0.68
1:B:665:THR:HG23	6:B:5418:HOH:O	1.93	0.68
1:B:502:ALA:CB	1:B:592:ILE:HD11	2.24	0.67
1:D:591[A]:GLU:OE1	5:D:5006:F6R:H1C1	1.95	0.67
1:B:571:LEU:HG	1:B:617:LEU:HD21	1.76	0.66
1:A:376:GLU:CD	1:A:376:GLU:H	2.00	0.66
1:A:428:GLU:OE1	1:A:436[A]:ARG:NH2	2.26	0.64
1:D:631:LYS:HE2	6:D:5188:HOH:O	1.99	0.63
1:C:691:LEU:O	1:C:695:ARG:HD2	1.98	0.63
1:B:418:GLU:OE2	6:B:5682:HOH:O	2.15	0.63
1:A:502:ALA:HB2	1:A:592:ILE:HD11	1.80	0.62
1:A:645:ARG:HE	1:A:662:VAL:HG11	1.64	0.62
1:A:502:ALA:CB	1:A:592:ILE:HD11	2.31	0.60
1:A:367:ASN:OD1	1:A:370:ARG:NH2	2.34	0.60
1:A:596:HIS:CD2	1:B:609:ILE:HD12	2.36	0.60
1:D:660:ASP:O	6:D:5114:HOH:O	2.17	0.59
1:B:571:LEU:HD21	6:B:5738:HOH:O	2.03	0.59
1:A:459:ILE:CD1	1:A:483:MET:HG2	2.34	0.58
1:C:451[B]:GLN:CD	1:C:477:ASN:HB2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HD13	1:A:483:MET:HG2	1.87	0.57
1:D:502:ALA:HB2	1:D:592:ILE:HD11	1.87	0.56
1:D:386:LYS:HE2	6:D:5012:HOH:O	2.05	0.56
1:D:350:TYR:CD2	1:D:356:LYS:HE3	2.40	0.56
1:D:587:LEU:HD12	1:D:591[B]:GLU:HG3	1.87	0.55
1:A:422:GLU:OE2	1:A:528:ARG:NH2	2.39	0.55
1:C:566:ASP:OD1	1:C:566:ASP:N	2.36	0.55
1:C:502:ALA:HB2	1:C:592:ILE:HD11	1.84	0.54
1:B:525:SER:OG	1:B:528:ARG:HG2	2.07	0.54
1:A:571:LEU:HG	1:A:617:LEU:CD2	2.37	0.54
1:A:395:CYS:HB3	1:C:442[B]:ARG:HH12	1.68	0.53
1:C:637:GLU:HG3	6:C:5626:HOH:O	2.08	0.53
1:B:459:ILE:CD1	1:B:483:MET:SD	2.83	0.53
1:C:502:ALA:CB	1:C:592:ILE:CD1	2.76	0.52
1:C:637:GLU:O	1:C:640:THR:HG22	2.08	0.52
1:B:613:VAL:O	1:B:642:ARG:NH2	2.43	0.52
1:C:544:GLU:HG3	6:C:5568:HOH:O	2.10	0.52
1:C:451[B]:GLN:CD	1:C:506:ALA:HB1	2.30	0.52
1:D:572:LEU:HD21	1:D:684:LEU:HD11	1.92	0.51
1:D:570:LEU:HD21	1:D:620:ILE:HD12	1.93	0.51
1:C:493:ILE:HD12	1:C:509[B]:SER:OG	2.10	0.51
1:A:571:LEU:HG	1:A:617:LEU:HD22	1.93	0.51
1:B:396:ARG:HD3	6:D:5077:HOH:O	2.11	0.51
1:A:569:SER:OG	1:A:596:HIS:ND1	2.38	0.50
1:A:526:ILE:CD1	1:D:526:ILE:HG12	2.40	0.50
1:C:609:ILE:O	1:C:613:VAL:HG13	2.11	0.50
1:B:417:PHE:HB3	1:B:425:VAL:HG21	1.93	0.50
1:C:417:PHE:HB3	1:C:425:VAL:HG21	1.94	0.49
1:C:462:LEU:HD22	1:C:483[A]:MET:CE	2.42	0.49
6:A:5727:HOH:O	1:C:394:ARG:HG2	2.13	0.49
1:B:525:SER:CB	1:B:528:ARG:HG2	2.42	0.49
4:A:5002:UD1:H5'2	4:A:5002:UD1:H8'2	1.94	0.49
1:B:392:ILE:HG23	1:B:445:THR:HG21	1.95	0.49
1:A:575:ARG:HD3	1:B:435:ASP:OD2	2.13	0.48
1:A:443:ASP:CG	6:A:5727:HOH:O	2.51	0.48
4:C:5004:UD1:H8'2	4:C:5004:UD1:H5'2	1.95	0.48
4:D:5005:UD1:H8'2	4:D:5005:UD1:H5'2	1.95	0.48
1:B:503:SER:O	1:B:588:LYS:CE	2.62	0.48
1:A:519:LEU:O	1:A:532:HIS:HE1	1.96	0.47
1:A:450:SER:O	1:A:476:VAL:HA	2.14	0.47
1:D:551:LYS:CE	6:D:5198:HOH:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLU:O	1:D:360:GLU:HG2	2.13	0.47
1:D:571:LEU:HG	1:D:617:LEU:HD11	1.97	0.46
1:D:569:SER:O	1:D:618:PRO:HD2	2.15	0.46
1:A:376:GLU:N	1:A:376:GLU:CD	2.67	0.46
1:C:396:ARG:HD3	6:C:5164:HOH:O	2.14	0.46
1:B:545:GLN:O	1:B:549:VAL:HG23	2.16	0.46
1:C:462:LEU:HD22	1:C:483[A]:MET:HE3	1.98	0.46
1:B:459:ILE:HD11	1:B:483:MET:HG2	1.98	0.46
1:A:529:LYS:O	1:A:533:GLU:HG3	2.16	0.46
1:B:360:GLU:HG2	1:B:360:GLU:O	2.15	0.45
6:A:5727:HOH:O	1:C:394:ARG:CG	2.64	0.45
1:D:417:PHE:HB3	1:D:425:VAL:HG21	1.98	0.45
1:C:544:GLU:CG	6:C:5568:HOH:O	2.63	0.45
1:D:453:GLY:O	1:D:483:MET:HG2	2.16	0.45
1:C:573:LEU:HD23	1:C:600:VAL:HB	1.97	0.45
1:B:367:ASN:OD1	1:B:370:ARG:NH2	2.49	0.45
1:A:405:THR:OG1	5:A:5003:F6R:H1C2	2.16	0.45
1:A:417:PHE:HB3	1:A:425:VAL:HG21	1.98	0.45
1:C:658:SER:HB2	1:C:661:LYS:H	1.82	0.45
1:C:609:ILE:HD12	1:D:596:HIS:CD2	2.52	0.45
1:B:450:SER:O	1:B:476:VAL:HA	2.17	0.45
1:A:459:ILE:CD1	1:A:483:MET:CG	2.95	0.44
1:A:573:LEU:HD23	1:A:600:VAL:HB	1.98	0.44
1:D:502:ALA:CB	1:D:592:ILE:HD11	2.46	0.44
1:B:569:SER:HA	1:B:596:HIS:O	2.18	0.44
1:B:519:LEU:O	1:B:532:HIS:HE1	2.01	0.43
1:C:645:ARG:O	1:C:645:ARG:HD3	2.18	0.43
1:D:682:ILE:HB	1:D:683:PRO:HD3	2.01	0.43
1:D:367:ASN:OD1	1:D:370:ARG:CZ	2.66	0.43
1:D:551:LYS:HE2	6:D:5198:HOH:O	2.18	0.43
1:C:450:SER:O	1:C:476[A]:VAL:HA	2.19	0.43
1:C:422:GLU:OE2	1:C:528:ARG:NH2	2.50	0.43
1:C:393:ARG:NH2	1:C:523:ASN:OD1	2.51	0.43
1:C:560:CYS:HA	1:C:564:LEU:HB2	2.00	0.42
1:D:476:VAL:O	1:D:492:HIS:HA	2.19	0.42
1:C:414:ARG:O	1:C:418:GLU:HG3	2.19	0.42
1:D:519:LEU:O	1:D:532:HIS:HE1	2.02	0.42
1:A:569:SER:O	1:A:618:PRO:HD2	2.19	0.42
1:C:657:ILE:HG13	1:C:663:HIS:CE1	2.55	0.42
1:C:571:LEU:HD11	1:C:609:ILE:HD11	2.01	0.42
1:B:570:LEU:HD22	1:B:589:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:O	1:B:597:SER:HA	2.20	0.42
1:A:519:LEU:O	1:A:532:HIS:CE1	2.73	0.42
1:C:450:SER:O	1:C:476[B]:VAL:HA	2.20	0.41
1:C:570:LEU:HB2	1:C:618:PRO:HB2	2.01	0.41
1:C:519:LEU:O	1:C:532:HIS:HE1	2.04	0.41
1:D:519:LEU:O	1:D:532:HIS:CE1	2.74	0.41
1:D:569:SER:HB2	1:D:596:HIS:ND1	2.35	0.41
1:D:680:ASN:O	1:D:683:PRO:HD2	2.20	0.41
1:C:671:THR:CG2	1:C:676:GLN:HA	2.51	0.41
1:C:502:ALA:HB1	1:C:588:LYS:HE2	2.01	0.41
1:D:418[A]:GLU:HG3	1:D:425:VAL:HB	2.01	0.41
1:B:442[B]:ARG:NH2	1:D:395:CYS:HB3	2.35	0.41
1:B:570:LEU:HD21	1:B:620:ILE:HD12	2.04	0.40
1:D:551:LYS:HE3	6:D:5198:HOH:O	2.21	0.40
1:A:503:SER:O	1:A:588:LYS:CE	2.69	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	335/367 (91%)	331 (99%)	4 (1%)	0	100	100
1	B	352/367 (96%)	346 (98%)	5 (1%)	1 (0%)	46	35
1	C	350/367 (95%)	345 (99%)	5 (1%)	0	100	100
1	D	341/367 (93%)	339 (99%)	2 (1%)	0	100	100
All	All	1378/1468 (94%)	1361 (99%)	16 (1%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	LYS

### 5.3.2 Protein sidechains ⓘ

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	297/319 (93%)	290 (98%)	7 (2%)	57	49
1	B	308/319 (97%)	302 (98%)	6 (2%)	65	59
1	C	310/319 (97%)	298 (96%)	12 (4%)	39	27
1	D	301/319 (94%)	295 (98%)	6 (2%)	63	57
All	All	1216/1276 (95%)	1185 (98%)	31 (2%)	55	47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	GLU
1	A	397	ARG
1	A	511	TYR
1	A	532	HIS
1	A	617	LEU
1	A	642	ARG
1	A	657	ILE
1	B	397[A]	ARG
1	B	397[B]	ARG
1	B	417	PHE
1	B	451	GLN
1	B	511	TYR
1	B	563	SER
1	C	397	ARG
1	C	511	TYR
1	C	563	SER
1	C	566	ASP
1	C	571	LEU
1	C	588	LYS
1	C	614	ASP
1	C	615	GLU

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Mol	Chain	Res	Type
1	C	640	THR
1	C	642	ARG
1	C	645	ARG
1	C	660	ASP
1	D	356	LYS
1	D	397	ARG
1	D	417	PHE
1	D	511	TYR
1	D	532	HIS
1	D	617	LEU

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

Mol	Chain	Res	Type
1	D	377	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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
4	UD1	A	5002	3	32,41,41	0.73	1 (3%)	46,62,62	1.55	1 (2%)
5	F6R	A	5003	-	15,15,15	0.88	0	14,21,21	1.33	2 (14%)
2	ACT	A	713	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
4	UD1	B	5003	3	32,41,41	0.88	1 (3%)	46,62,62	1.45	5 (10%)
5	F6R	B	5004	-	15,15,15	0.70	0	14,21,21	1.50	3 (21%)
4	UD1	C	5004	3	32,41,41	0.80	2 (6%)	46,62,62	1.73	3 (6%)
5	F6R	C	5005	-	15,15,15	0.99	1 (6%)	14,21,21	0.93	1 (7%)
2	ACT	C	713	-	1,3,3	2.49	1 (100%)	0,3,3	0.00	-
4	UD1	D	5005	3	32,41,41	0.80	1 (3%)	46,62,62	1.44	3 (6%)
5	F6R	D	5006	-	15,15,15	1.17	2 (13%)	14,21,21	1.31	2 (14%)

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
4	UD1	A	5002	3	-	0/22/63/63	0/3/3/3
5	F6R	A	5003	-	-	0/20/20/20	0/0/0/0
2	ACT	A	713	-	-	0/0/0/0	0/0/0/0
4	UD1	B	5003	3	-	0/22/63/63	0/3/3/3
5	F6R	B	5004	-	-	0/20/20/20	0/0/0/0
4	UD1	C	5004	3	-	0/22/63/63	0/3/3/3
5	F6R	C	5005	-	-	0/20/20/20	0/0/0/0
2	ACT	C	713	-	-	0/0/0/0	0/0/0/0
4	UD1	D	5005	3	-	0/22/63/63	0/3/3/3
5	F6R	D	5006	-	-	0/20/20/20	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5006	F6R	P-O1P	-2.09	1.47	1.54
4	C	5004	UD1	PB-O2B	-2.09	1.46	1.54
2	A	713	ACT	CH3-C	2.24	1.51	1.48
5	D	5006	F6R	P-O3P	2.31	1.58	1.51
2	C	713	ACT	CH3-C	2.49	1.52	1.48
5	C	5005	F6R	P-O3P	2.65	1.59	1.51
4	A	5002	UD1	O4B-C1B	2.71	1.44	1.41
4	C	5004	UD1	O4B-C1B	2.90	1.44	1.41
4	D	5005	UD1	O4B-C1B	3.54	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5003	UD1	O4B-C1B	3.84	1.46	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5004	F6R	O3-C3-C4	-2.62	104.95	110.41
5	A	5003	F6R	O4-C4-C3	-2.60	104.58	109.28
5	D	5006	F6R	O3-C3-C2	-2.54	106.30	111.01
4	C	5004	UD1	O6'-C6'-C5'	-2.36	103.54	111.33
4	D	5005	UD1	O3A-PA-O5B	-2.21	97.08	102.94
5	C	5005	F6R	O1-C1-C2	-2.16	106.85	112.66
4	B	5003	UD1	O3A-PA-O5B	-2.07	97.44	102.94
4	B	5003	UD1	PB-O3A-PA	-2.04	126.99	132.73
4	C	5004	UD1	PB-O3A-PA	-2.04	127.00	132.73
5	B	5004	F6R	O1-C1-C2	-2.02	107.21	112.66
5	A	5003	F6R	O1P-P-O6	2.02	112.38	106.56
4	D	5005	UD1	C4'-C3'-C2'	2.07	113.30	110.43
4	B	5003	UD1	O2B-PB-O1'	2.08	114.85	106.49
4	B	5003	UD1	O5'-C5'-C4'	2.20	113.81	109.68
5	D	5006	F6R	O1P-P-O3P	2.24	117.80	110.58
5	B	5004	F6R	O1P-P-O6	3.32	116.13	106.56
4	D	5005	UD1	C4-N3-C2	6.57	120.64	114.14
4	B	5003	UD1	C4-N3-C2	7.13	121.20	114.14
4	A	5002	UD1	C4-N3-C2	8.39	122.45	114.14
4	C	5004	UD1	C4-N3-C2	9.92	123.97	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5002	UD1	1	0
5	A	5003	F6R	1	0
5	B	5004	F6R	1	0
4	C	5004	UD1	1	0
5	C	5005	F6R	1	0
4	D	5005	UD1	1	0
5	D	5006	F6R	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	339/367 (92%)	-0.01	14 (4%) 41 45	12, 22, 40, 53	0
1	B	352/367 (95%)	0.00	13 (3%) 45 49	14, 22, 46, 58	0
1	C	350/367 (95%)	0.11	22 (6%) 23 26	13, 24, 50, 63	0
1	D	341/367 (92%)	-0.07	13 (3%) 44 48	13, 22, 37, 47	0
All	All	1382/1468 (94%)	0.01	62 (4%) 37 40	12, 22, 44, 63	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	ILE	5.3
1	C	615	GLU	5.2
1	C	660	ASP	5.1
1	D	499	ILE	4.5
1	C	594	TYR	4.4
1	B	594	TYR	4.3
1	A	658	SER	4.1
1	B	607	HIS	4.0
1	C	607	HIS	4.0
1	A	642	ARG	4.0
1	B	499	ILE	4.0
1	A	501	VAL	3.9
1	B	566	ASP	3.7
1	C	655	ALA	3.7
1	D	376	GLU	3.7
1	B	386	LYS	3.7
1	A	349	PRO	3.6
1	D	659	ASN	3.5
1	C	662	VAL	3.5
1	A	606	LYS	3.5
1	A	563	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	642	ARG	3.4
1	D	605	LEU	3.3
1	C	499	ILE	3.3
1	A	655	ALA	3.3
1	C	606	LYS	3.1
1	B	606	LYS	3.1
1	C	611	ALA	2.9
1	C	661	LYS	2.9
1	C	643	ASP	2.9
1	D	617	LEU	2.9
1	A	641	ALA	2.9
1	B	353	PHE	2.9
1	C	353	PHE	2.9
1	D	349	PRO	2.9
1	D	386	LYS	2.8
1	D	642	ARG	2.8
1	B	563	SER	2.7
1	C	376	GLU	2.7
1	C	616	ASP	2.7
1	A	353	PHE	2.7
1	A	662	VAL	2.6
1	B	376	GLU	2.6
1	C	568	LYS	2.6
1	C	696	GLY	2.6
1	A	617	LEU	2.6
1	C	613	VAL	2.6
1	D	353	PHE	2.5
1	C	349	PRO	2.4
1	B	596	HIS	2.4
1	C	641	ALA	2.4
1	D	568	LYS	2.4
1	B	349	PRO	2.2
1	B	351	LYS	2.2
1	A	657	ILE	2.2
1	C	658	SER	2.1
1	A	387	SER	2.1
1	C	596	HIS	2.0
1	B	565	ASN	2.0
1	D	563	SER	2.0
1	D	658	SER	2.0
1	D	603	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
5	F6R	C	5005	16/16	0.97	0.12	0.88	22,30,39,44	0
2	ACT	C	713	4/4	0.94	0.14	0.29	32,32,33,34	0
4	UD1	B	5003	39/39	0.95	0.12	0.24	16,24,53,56	0
2	ACT	A	713	4/4	0.91	0.12	0.04	32,32,33,33	0
5	F6R	A	5003	16/16	0.98	0.10	0.03	17,22,30,30	0
4	UD1	D	5005	39/39	0.94	0.12	-0.04	17,24,44,46	0
5	F6R	B	5004	16/16	0.97	0.09	-0.08	15,22,36,36	0
4	UD1	A	5002	39/39	0.94	0.12	-0.11	18,24,45,50	0
4	UD1	C	5004	39/39	0.97	0.09	-0.51	14,23,28,37	0
3	NA	B	5002	1/1	0.99	0.07	-0.53	19,19,19,19	0
3	NA	A	5001	1/1	0.97	0.08	-0.82	20,20,20,20	0
5	F6R	D	5006	16/16	0.98	0.06	-0.92	18,23,27,28	0
3	NA	D	5004	1/1	0.97	0.06	-1.54	23,23,23,23	0
3	NA	C	5003	1/1	0.98	0.04	-2.74	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.