



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2016 – 10:21 PM EDT

PDB ID : 5IN5  
Title : Crystal Structure of GDP-mannose 4,6 dehydratase in complex with natural inhibitor GDP-Fucose  
Authors : Sickmier, E.A.  
Deposited on : 2016-03-07  
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.

---

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

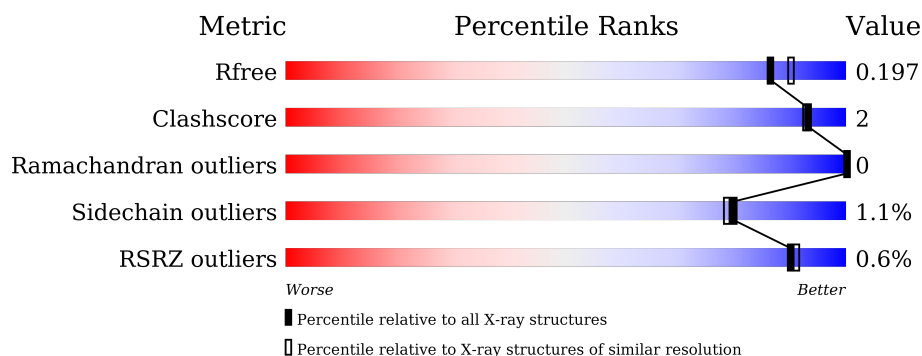
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	364	<div> <div>%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	B	364	<div> <div>%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	C	364	<div> <div></div> <div>93%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div>
1	D	364	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> <div> <div></div> <div></div> <div></div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13281 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 GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	2	0
			2822	1799	486	527	10			
1	B	351	Total	C	N	O	S	0	3	0
			2823	1798	487	526	12			
1	C	355	Total	C	N	O	S	0	1	0
			2858	1824	491	533	10			
1	D	351	Total	C	N	O	S	0	0	0
			2812	1791	486	525	10			

There are 56 discrepancies between the modelled and reference sequences:

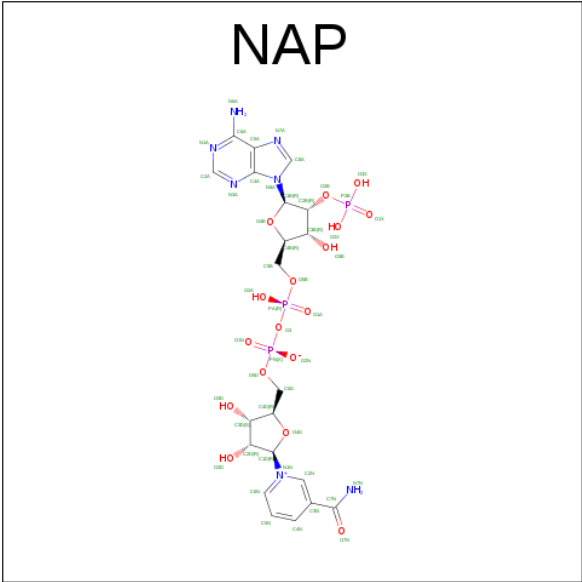
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP O60547
A	10	HIS	-	expression tag	UNP O60547
A	11	HIS	-	expression tag	UNP O60547
A	12	HIS	-	expression tag	UNP O60547
A	13	HIS	-	expression tag	UNP O60547
A	14	HIS	-	expression tag	UNP O60547
A	15	HIS	-	expression tag	UNP O60547
A	16	GLU	-	expression tag	UNP O60547
A	17	ASN	-	expression tag	UNP O60547
A	18	LEU	-	expression tag	UNP O60547
A	19	TYR	-	expression tag	UNP O60547
A	20	PHE	-	expression tag	UNP O60547
A	21	GLN	-	expression tag	UNP O60547
A	22	GLY	-	expression tag	UNP O60547
B	9	MET	-	expression tag	UNP O60547
B	10	HIS	-	expression tag	UNP O60547
B	11	HIS	-	expression tag	UNP O60547
B	12	HIS	-	expression tag	UNP O60547
B	13	HIS	-	expression tag	UNP O60547
B	14	HIS	-	expression tag	UNP O60547
B	15	HIS	-	expression tag	UNP O60547

*Continued on next page...*

*Continued from previous page...*

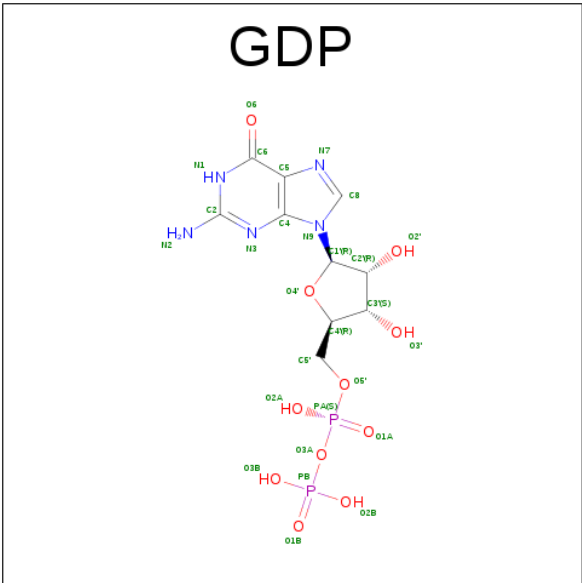
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	GLU	-	expression tag	UNP O60547
B	17	ASN	-	expression tag	UNP O60547
B	18	LEU	-	expression tag	UNP O60547
B	19	TYR	-	expression tag	UNP O60547
B	20	PHE	-	expression tag	UNP O60547
B	21	GLN	-	expression tag	UNP O60547
B	22	GLY	-	expression tag	UNP O60547
C	9	MET	-	expression tag	UNP O60547
C	10	HIS	-	expression tag	UNP O60547
C	11	HIS	-	expression tag	UNP O60547
C	12	HIS	-	expression tag	UNP O60547
C	13	HIS	-	expression tag	UNP O60547
C	14	HIS	-	expression tag	UNP O60547
C	15	HIS	-	expression tag	UNP O60547
C	16	GLU	-	expression tag	UNP O60547
C	17	ASN	-	expression tag	UNP O60547
C	18	LEU	-	expression tag	UNP O60547
C	19	TYR	-	expression tag	UNP O60547
C	20	PHE	-	expression tag	UNP O60547
C	21	GLN	-	expression tag	UNP O60547
C	22	GLY	-	expression tag	UNP O60547
D	9	MET	-	expression tag	UNP O60547
D	10	HIS	-	expression tag	UNP O60547
D	11	HIS	-	expression tag	UNP O60547
D	12	HIS	-	expression tag	UNP O60547
D	13	HIS	-	expression tag	UNP O60547
D	14	HIS	-	expression tag	UNP O60547
D	15	HIS	-	expression tag	UNP O60547
D	16	GLU	-	expression tag	UNP O60547
D	17	ASN	-	expression tag	UNP O60547
D	18	LEU	-	expression tag	UNP O60547
D	19	TYR	-	expression tag	UNP O60547
D	20	PHE	-	expression tag	UNP O60547
D	21	GLN	-	expression tag	UNP O60547
D	22	GLY	-	expression tag	UNP O60547

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



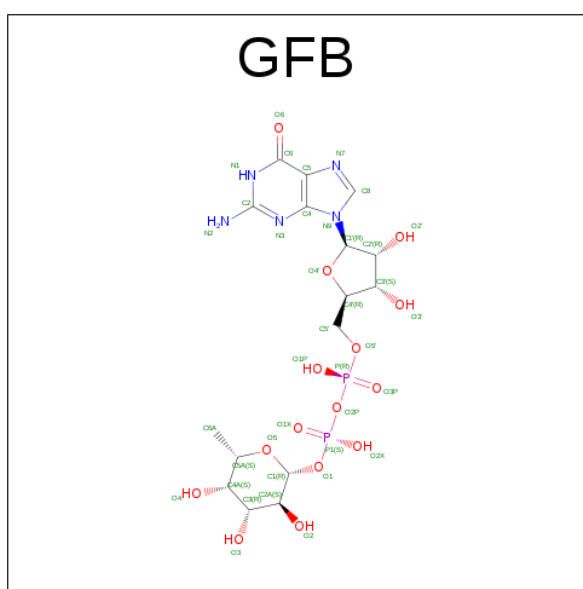
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE-BETA-L-FUCOPYRANOSE (three-letter code: GFB) (formula:  $C_{16}H_{25}N_5O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
4	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
4	C	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
4	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	377	Total	O	0	0
			377	377		
6	B	385	Total	O	0	0
			385	385		
6	C	388	Total	O	0	0
			388	388		
6	D	354	Total	O	0	0
			354	354		

### 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: GDP-mannose 4,6 dehydratase



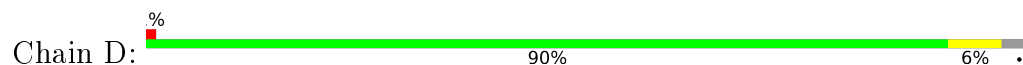
- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.14Å 140.16Å 86.03Å 90.00° 106.32° 90.00°	Depositor
Resolution (Å)	19.89 – 1.90 19.89 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.89-1.90) 94.5 (19.89-1.89)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.149 , 0.198 0.148 , 0.197	Depositor DCC
$R_{free}$ test set	5336 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: GDP, GOL, NAP, GFB

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	0.38	0/2891	0.53	0/3911
1	B	0.37	0/2895	0.52	0/3916
1	C	0.37	0/2926	0.50	0/3958
1	D	0.37	0/2875	0.51	0/3889
All	All	0.37	0/11587	0.52	0/15674

There are no bond length outliers.

There are no bond angle outliers.

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	2822	0	2790	11	0
1	B	2823	0	2791	12	0
1	C	2858	0	2818	7	0
1	D	2812	0	2775	14	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	28	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	38	0	23	0	0
4	B	38	0	22	0	0
4	C	38	0	23	0	0
4	D	38	0	22	0	0
5	A	6	0	8	0	0
6	A	377	0	0	3	1
6	B	385	0	0	2	0
6	C	388	0	0	2	0
6	D	354	0	0	4	1
All	All	13281	0	11420	43	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 2.

All (43) 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:D:291:HIS:NE2	1:D:356:ARG:HG2	2.06	0.70
1:B:352:ASP:HB3	1:B:356:ARG:HH22	1.60	0.66
1:A:81:LYS:NZ	6:A:1104:HOH:O	2.31	0.63
1:C:120:LEU:HG	1:C:123:TYR:HB3	1.84	0.60
1:B:352:ASP:HB3	1:B:356:ARG:NH2	2.18	0.58
1:D:291:HIS:CE1	1:D:356:ARG:HG2	2.39	0.56
1:B:119:ASP:OD1	6:B:501:HOH:O	2.17	0.56
1:C:41:GLU:O	1:C:45:GLU:HG3	2.05	0.56
1:B:120:LEU:HG	1:B:123:TYR:HB3	1.87	0.55
1:D:234:GLN:OE1	6:D:501:HOH:O	2.18	0.54
1:D:352:ASP:O	1:D:356:ARG:HG3	2.08	0.53
1:A:291:HIS:CE1	1:A:356:ARG:HB2	2.45	0.52
1:C:62:THR:O	1:C:66[B]:GLU:HG3	2.10	0.52
1:D:120:LEU:HG	1:D:123:TYR:HB3	1.92	0.52
1:B:283:GLU:OE1	6:B:502:HOH:O	2.19	0.52
1:B:282:ARG:NH2	1:B:305:GLU:OE2	2.39	0.51
1:B:184:LEU:HG	1:D:184:LEU:HD21	1.92	0.51
1:D:144:LEU:HB3	1:D:148:VAL:HG23	1.95	0.49
1:A:120:LEU:HG	1:A:123:TYR:HB3	1.95	0.48
1:A:23:ARG:NH1	6:A:1109:HOH:O	2.33	0.48
1:C:348:ARG:HD2	6:C:1245:HOH:O	2.14	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:OE1	1:C:342:LYS:NZ	2.45	0.47
1:A:291:HIS:NE2	1:A:356:ARG:HB2	2.29	0.47
1:B:291:HIS:NE2	1:B:356:ARG:HG2	2.30	0.47
1:C:257:GLU:OE1	6:C:1101:HOH:O	2.21	0.46
1:B:123:TYR:CZ	1:B:127:VAL:HG21	2.51	0.45
1:A:51:HIS:CE1	1:A:81:LYS:HD2	2.52	0.45
1:A:66[B]:GLU:HG2	6:A:1191:HOH:O	2.17	0.44
1:D:149:LYS:HB3	1:D:263:LEU:HG	1.99	0.44
1:D:99:GLU:HG3	6:D:691:HOH:O	2.18	0.43
1:B:352:ASP:O	1:B:356:ARG:HG3	2.17	0.43
1:C:50:VAL:O	1:C:80:MET:HA	2.18	0.43
1:D:160:GLY:HA3	1:D:174:TYR:O	2.19	0.42
1:D:98:ASN:OD1	6:D:502:HOH:O	2.21	0.42
1:A:123:TYR:CZ	1:A:127:VAL:HG21	2.54	0.42
1:B:113:HIS:CE1	1:B:115:LYS:HB3	2.55	0.42
1:A:22:GLY:HA2	1:A:23:ARG:HA	1.68	0.41
1:A:362:ASP:O	1:A:366:MET:HG2	2.20	0.41
1:D:161:LYS:NZ	6:D:511:HOH:O	2.33	0.41
1:B:160:GLY:HA3	1:B:174:TYR:O	2.21	0.41
1:D:231:TYR:CD1	1:D:292:ILE:HB	2.56	0.41
1:D:362:ASP:O	1:D:366:MET:HG2	2.21	0.40
1:A:280:SER:OG	1:A:283:GLU:HG3	2.21	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)
6:A:1226:HOH:O	6:D:734:HOH:O[2_345]	2.16	0.04

## 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	351/364 (96%)	343 (98%)	8 (2%)	0	100	100
1	B	352/364 (97%)	345 (98%)	7 (2%)	0	100	100
1	C	354/364 (97%)	349 (99%)	5 (1%)	0	100	100
1	D	349/364 (96%)	342 (98%)	7 (2%)	0	100	100
All	All	1406/1456 (97%)	1379 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	304/315 (96%)	300 (99%)	4 (1%)	76	73
1	B	305/315 (97%)	301 (99%)	4 (1%)	76	73
1	C	307/315 (98%)	303 (99%)	4 (1%)	76	73
1	D	302/315 (96%)	300 (99%)	2 (1%)	88	88
All	All	1218/1260 (97%)	1204 (99%)	14 (1%)	80	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	CYS
1	A	111	GLN
1	A	174	TYR
1	A	356	ARG
1	B	92[A]	CYS
1	B	92[B]	CYS
1	B	111	GLN
1	B	356	ARG
1	C	60	PHE
1	C	92	CYS
1	C	111	GLN
1	C	210	GLU
1	D	92	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	111	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	21	GLN
1	C	341	GLN
1	D	98	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](#)

13 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	NAP	A	1001	-	45,52,52	1.75	9 (20%)	55,80,80	1.96	15 (27%)
3	GDP	A	1002	-	24,30,30	1.05	2 (8%)	26,47,47	1.75	6 (23%)
4	GFB	A	1003	-	35,41,41	2.69	11 (31%)	44,64,64	1.72	8 (18%)
5	GOL	A	1004	-	5,5,5	0.34	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GFB	B	401	-	35,41,41	2.80	11 (31%)	44,64,64	1.60	7 (15%)
2	NAP	B	402	-	45,52,52	2.02	9 (20%)	55,80,80	1.94	16 (29%)
3	GDP	B	403	-	24,30,30	1.00	2 (8%)	26,47,47	1.87	5 (19%)
2	NAP	C	1001	-	45,52,52	2.07	12 (26%)	55,80,80	1.96	11 (20%)
3	GDP	C	1002	-	24,30,30	1.14	2 (8%)	26,47,47	1.89	5 (19%)
4	GFB	C	1003	-	35,41,41	2.66	11 (31%)	44,64,64	1.78	10 (22%)
4	GFB	D	401	-	35,41,41	2.79	10 (28%)	44,64,64	1.61	8 (18%)
2	NAP	D	402	-	45,52,52	2.00	12 (26%)	55,80,80	1.92	12 (21%)
3	GDP	D	403	-	24,30,30	1.13	2 (8%)	26,47,47	1.86	4 (15%)

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	NAP	A	1001	-	-	0/27/67/67	0/5/5/5
3	GDP	A	1002	-	-	0/12/32/32	0/3/3/3
4	GFB	A	1003	-	-	0/17/57/57	0/4/4/4
5	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
4	GFB	B	401	-	-	0/17/57/57	0/4/4/4
2	NAP	B	402	-	-	0/27/67/67	0/5/5/5
3	GDP	B	403	-	-	0/12/32/32	0/3/3/3
2	NAP	C	1001	-	-	0/27/67/67	0/5/5/5
3	GDP	C	1002	-	-	0/12/32/32	0/3/3/3
4	GFB	C	1003	-	-	0/17/57/57	0/4/4/4
4	GFB	D	401	-	-	0/17/57/57	0/4/4/4
2	NAP	D	402	-	-	0/27/67/67	0/5/5/5
3	GDP	D	403	-	-	0/12/32/32	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	GFB	O4'-C1'	-8.78	1.28	1.41
4	D	401	GFB	O4'-C1'	-8.76	1.28	1.41
4	A	1003	GFB	O4'-C1'	-7.83	1.30	1.41
4	C	1003	GFB	O4'-C1'	-7.83	1.30	1.41
4	A	1003	GFB	C3'-C4'	-6.88	1.34	1.53
4	B	401	GFB	C3'-C4'	-6.80	1.34	1.53
4	D	401	GFB	C3'-C4'	-6.76	1.34	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	GFB	C3'-C4'	-6.68	1.35	1.53
2	D	402	NAP	C3N-C7N	-3.66	1.44	1.50
2	D	402	NAP	O2B-C2B	-3.52	1.33	1.44
4	D	401	GFB	O2'-C2'	-2.98	1.35	1.43
2	C	1001	NAP	O2B-C2B	-2.89	1.34	1.44
4	B	401	GFB	O2'-C2'	-2.82	1.36	1.43
2	C	1001	NAP	C3N-C7N	-2.74	1.46	1.50
2	B	402	NAP	C3N-C7N	-2.63	1.46	1.50
2	A	1001	NAP	O2B-C2B	-2.56	1.36	1.44
4	A	1003	GFB	O2'-C2'	-2.51	1.37	1.43
2	B	402	NAP	O2B-C2B	-2.50	1.36	1.44
4	C	1003	GFB	O2'-C2'	-2.46	1.37	1.43
2	D	402	NAP	C6N-C5N	-2.25	1.33	1.38
2	A	1001	NAP	C3N-C7N	-2.24	1.47	1.50
4	D	401	GFB	C2A-C3	-2.23	1.46	1.52
2	C	1001	NAP	C6N-C5N	-2.22	1.33	1.38
4	C	1003	GFB	C2A-C3	-2.21	1.46	1.52
4	D	401	GFB	O6-C6	-2.21	1.19	1.24
4	A	1003	GFB	C2A-C3	-2.10	1.46	1.52
4	B	401	GFB	C2A-C3	-2.07	1.46	1.52
2	A	1001	NAP	O5D-C5D	-2.04	1.36	1.44
4	C	1003	GFB	C2'-C1'	2.05	1.56	1.53
4	A	1003	GFB	C2'-C1'	2.15	1.57	1.53
2	C	1001	NAP	C6N-N1N	2.16	1.41	1.35
2	C	1001	NAP	C2D-C1D	2.17	1.57	1.53
4	B	401	GFB	C2'-C1'	2.19	1.57	1.53
2	B	402	NAP	C2D-C1D	2.19	1.57	1.53
2	B	402	NAP	C6N-N1N	2.20	1.41	1.35
2	D	402	NAP	C2D-C1D	2.29	1.57	1.53
2	D	402	NAP	C6N-N1N	2.34	1.42	1.35
4	C	1003	GFB	O5-C1	2.34	1.47	1.41
4	B	401	GFB	O3-C3	2.35	1.48	1.43
4	C	1003	GFB	O3-C3	2.37	1.48	1.43
2	D	402	NAP	C4A-N3A	2.38	1.39	1.35
4	A	1003	GFB	O5-C1	2.45	1.48	1.41
4	A	1003	GFB	O3-C3	2.47	1.48	1.43
2	A	1001	NAP	C2A-N1A	2.48	1.38	1.33
2	D	402	NAP	C2A-N1A	2.48	1.38	1.33
4	D	401	GFB	O5-C1	2.56	1.48	1.41
4	B	401	GFB	O5-C1	2.59	1.48	1.41
3	B	403	GDP	C5-C4	2.64	1.46	1.40
2	C	1001	NAP	C4A-N3A	2.70	1.39	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	GFB	O3'-C3'	2.74	1.49	1.43
2	A	1001	NAP	C2N-N1N	2.77	1.39	1.35
3	A	1002	GDP	C5-C4	2.82	1.46	1.40
2	C	1001	NAP	PN-O5D	2.84	1.71	1.59
4	D	401	GFB	P1-O1	2.86	1.68	1.60
3	B	403	GDP	C6-C5	2.88	1.47	1.41
4	C	1003	GFB	P1-O1	2.91	1.68	1.60
4	C	1003	GFB	O3'-C3'	2.94	1.49	1.43
4	A	1003	GFB	O3'-C3'	2.94	1.49	1.43
3	C	1002	GDP	C5-C4	2.98	1.47	1.40
2	D	402	NAP	C2N-N1N	2.99	1.39	1.35
2	C	1001	NAP	C2A-N1A	3.02	1.39	1.33
3	A	1002	GDP	C6-C5	3.09	1.47	1.41
2	A	1001	NAP	PN-O5D	3.11	1.72	1.59
4	A	1003	GFB	P1-O1	3.14	1.69	1.60
3	D	403	GDP	C5-C4	3.20	1.47	1.40
4	B	401	GFB	P1-O1	3.24	1.69	1.60
2	B	402	NAP	C2N-N1N	3.30	1.39	1.35
3	D	403	GDP	C6-C5	3.38	1.48	1.41
4	D	401	GFB	O3'-C3'	3.39	1.51	1.43
3	C	1002	GDP	C6-C5	3.42	1.48	1.41
2	A	1001	NAP	C5N-C4N	3.42	1.45	1.38
2	C	1001	NAP	C2N-N1N	3.45	1.40	1.35
2	B	402	NAP	PN-O5D	3.57	1.74	1.59
2	A	1001	NAP	C7N-N7N	3.64	1.40	1.33
2	D	402	NAP	PN-O5D	3.84	1.75	1.59
2	D	402	NAP	C7N-N7N	4.07	1.41	1.33
2	D	402	NAP	C5N-C4N	4.18	1.47	1.38
2	B	402	NAP	C7N-N7N	4.32	1.41	1.33
2	C	1001	NAP	C7N-N7N	4.39	1.41	1.33
4	A	1003	GFB	C2-N2	4.48	1.43	1.34
2	C	1001	NAP	C5N-C4N	4.61	1.47	1.38
4	B	401	GFB	C2-N2	4.73	1.44	1.34
2	B	402	NAP	C5N-C4N	4.75	1.48	1.38
4	D	401	GFB	C2-N2	4.78	1.44	1.34
4	C	1003	GFB	C2-N2	4.80	1.44	1.34
2	A	1001	NAP	C4N-C3N	5.84	1.48	1.39
2	D	402	NAP	C4N-C3N	5.95	1.49	1.39
2	C	1001	NAP	C4N-C3N	6.73	1.50	1.39
2	B	402	NAP	C4N-C3N	6.82	1.50	1.39
4	C	1003	GFB	O4'-C4'	7.10	1.61	1.45
4	A	1003	GFB	O4'-C4'	7.14	1.61	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	GFB	O4'-C4'	7.26	1.61	1.45
4	D	401	GFB	O4'-C4'	7.31	1.61	1.45

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAP	C5N-C4N-C3N	-6.61	112.46	120.35
2	B	402	NAP	C5N-C4N-C3N	-6.53	112.56	120.35
2	C	1001	NAP	C5N-C4N-C3N	-6.29	112.84	120.35
2	D	402	NAP	C5N-C4N-C3N	-6.05	113.13	120.35
2	A	1001	NAP	O2B-P2B-O1X	-5.34	94.72	107.48
4	C	1003	GFB	O5-C1-O1	-5.03	104.73	111.36
4	A	1003	GFB	O5-C1-O1	-4.90	104.90	111.36
2	D	402	NAP	O2B-P2B-O1X	-4.83	95.94	107.48
2	C	1001	NAP	O2B-P2B-O1X	-4.67	96.32	107.48
2	B	402	NAP	O2B-P2B-O1X	-4.40	96.98	107.48
3	D	403	GDP	C5-C6-N1	-4.35	117.84	123.52
2	C	1001	NAP	O4D-C1D-N1N	-4.33	103.43	108.10
3	C	1002	GDP	C5-C6-N1	-4.25	117.97	123.52
2	C	1001	NAP	C4B-O4B-C1B	-4.13	105.27	109.64
4	D	401	GFB	N3-C2-N1	-4.11	121.96	127.56
4	C	1003	GFB	N3-C2-N1	-4.09	121.99	127.56
3	A	1002	GDP	C5-C6-N1	-4.00	118.30	123.52
3	B	403	GDP	N3-C2-N1	-3.96	122.17	127.56
3	D	403	GDP	N3-C2-N1	-3.95	122.19	127.56
4	B	401	GFB	N3-C2-N1	-3.93	122.21	127.56
4	A	1003	GFB	N3-C2-N1	-3.90	122.25	127.56
2	D	402	NAP	O4D-C1D-N1N	-3.87	103.92	108.10
4	A	1003	GFB	C4'-O4'-C1'	-3.84	105.57	109.64
3	B	403	GDP	C6-C5-C4	-3.77	116.55	120.86
3	C	1002	GDP	N3-C2-N1	-3.73	122.48	127.56
3	B	403	GDP	C5-C6-N1	-3.62	118.79	123.52
3	A	1002	GDP	N3-C2-N1	-3.50	122.80	127.56
4	C	1003	GFB	C5-C6-N1	-3.47	118.99	123.52
4	B	401	GFB	C1'-N9-C4	-3.43	122.97	126.81
4	B	401	GFB	O5-C1-O1	-3.39	106.90	111.36
4	A	1003	GFB	C5-C6-N1	-3.34	119.15	123.52
4	B	401	GFB	C5-C6-N1	-3.34	119.16	123.52
4	D	401	GFB	C5-C6-N1	-3.27	119.25	123.52
2	B	402	NAP	C4B-O4B-C1B	-3.26	106.19	109.64
4	C	1003	GFB	C4'-O4'-C1'	-3.25	106.20	109.64
4	D	401	GFB	C4'-O4'-C1'	-3.19	106.26	109.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	GDP	C6-C5-C4	-3.14	117.27	120.86
2	B	402	NAP	O7N-C7N-N7N	-3.07	118.21	122.58
2	B	402	NAP	O3X-P2B-O2B	-3.02	97.59	106.62
2	A	1001	NAP	O4D-C1D-N1N	-3.02	104.84	108.10
2	B	402	NAP	O4D-C1D-N1N	-2.98	104.89	108.10
2	D	402	NAP	C4B-O4B-C1B	-2.97	106.50	109.64
2	C	1001	NAP	C3B-C2B-C1B	-2.88	97.12	102.63
2	D	402	NAP	C3B-C2B-C1B	-2.87	97.13	102.63
4	C	1003	GFB	C1'-N9-C4	-2.85	123.62	126.81
3	D	403	GDP	C6-C5-C4	-2.77	117.69	120.86
2	C	1001	NAP	O7N-C7N-N7N	-2.76	118.64	122.58
2	B	402	NAP	C3B-C2B-C1B	-2.75	97.36	102.63
3	A	1002	GDP	C6-C5-C4	-2.74	117.72	120.86
4	D	401	GFB	O5-C1-O1	-2.74	107.75	111.36
2	A	1001	NAP	C4B-O4B-C1B	-2.73	106.75	109.64
2	A	1001	NAP	C3B-C2B-C1B	-2.67	97.52	102.63
4	B	401	GFB	C6-C5-C4	-2.65	117.83	120.86
2	C	1001	NAP	O3X-P2B-O2B	-2.54	99.04	106.62
2	A	1001	NAP	O7N-C7N-N7N	-2.51	119.01	122.58
2	D	402	NAP	O5D-PN-O1N	-2.43	99.27	109.21
2	B	402	NAP	P2B-O2B-C2B	-2.41	115.40	121.56
2	B	402	NAP	C2A-N1A-C6A	-2.41	114.47	118.77
4	D	401	GFB	C6-C5-C4	-2.38	118.14	120.86
4	D	401	GFB	C1'-N9-C4	-2.37	124.16	126.81
4	C	1003	GFB	C6-C5-C4	-2.35	118.17	120.86
2	A	1001	NAP	O3X-P2B-O2B	-2.35	99.60	106.62
2	A	1001	NAP	C2A-N1A-C6A	-2.35	114.58	118.77
2	D	402	NAP	O3X-P2B-O2B	-2.31	99.72	106.62
4	A	1003	GFB	C6-C5-C4	-2.31	118.22	120.86
4	A	1003	GFB	C1'-N9-C4	-2.29	124.25	126.81
4	C	1003	GFB	C1-O5-C5A	-2.27	109.60	113.76
2	D	402	NAP	O7N-C7N-N7N	-2.16	119.50	122.58
2	B	402	NAP	C1B-N9A-C4A	-2.10	124.47	126.81
2	A	1001	NAP	O5D-PN-O1N	-2.08	100.70	109.21
2	C	1001	NAP	C2A-N1A-C6A	-2.06	115.08	118.77
2	B	402	NAP	O2N-PN-O1N	2.03	123.10	112.56
3	A	1002	GDP	O4'-C1'-N9	2.06	111.99	108.11
2	A	1001	NAP	O2X-P2B-O1X	2.08	117.41	110.63
2	A	1001	NAP	N3A-C2A-N1A	2.09	130.51	128.87
4	C	1003	GFB	C2'-C3'-C4'	2.11	106.95	102.64
3	A	1002	GDP	O2A-PA-O3A	2.34	115.30	105.27
2	D	402	NAP	O7N-C7N-C3N	2.34	122.19	119.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	GDP	O4'-C1'-N9	2.36	112.57	108.11
2	B	402	NAP	N3A-C2A-N1A	2.41	130.76	128.87
2	A	1001	NAP	O3X-P2B-O2X	2.49	116.58	107.44
2	B	402	NAP	O3X-P2B-O2X	2.49	116.59	107.44
4	B	401	GFB	O2P-P1-O1	2.51	106.54	102.05
2	B	402	NAP	O2N-PN-O3	2.57	116.28	105.27
2	C	1001	NAP	O3X-P2B-O2X	2.60	116.97	107.44
2	D	402	NAP	O3X-P2B-O2X	2.60	116.98	107.44
3	B	403	GDP	O4'-C1'-N9	2.67	113.15	108.11
2	C	1001	NAP	O2N-PN-O3	2.76	117.08	105.27
2	A	1001	NAP	O7N-C7N-C3N	2.86	122.76	119.60
2	B	402	NAP	O7N-C7N-C3N	2.89	122.80	119.60
2	A	1001	NAP	O2N-PN-O3	2.92	117.77	105.27
2	D	402	NAP	O2N-PN-O3	2.97	117.98	105.27
4	A	1003	GFB	O2P-P1-O1	3.42	108.15	102.05
4	C	1003	GFB	O2P-P1-O1	3.46	108.22	102.05
2	B	402	NAP	C2N-C3N-C4N	3.63	122.39	118.27
2	C	1001	NAP	C2N-C3N-C4N	3.71	122.48	118.27
4	B	401	GFB	C6-N1-C2	3.90	120.45	115.88
4	A	1003	GFB	C6-N1-C2	3.96	120.52	115.88
4	D	401	GFB	C6-N1-C2	4.03	120.60	115.88
2	A	1001	NAP	C2N-C3N-C4N	4.12	122.94	118.27
4	D	401	GFB	O2P-P1-O1	4.13	109.43	102.05
4	C	1003	GFB	C6-N1-C2	4.20	120.80	115.88
2	D	402	NAP	C2N-C3N-C4N	4.49	123.36	118.27
3	A	1002	GDP	C6-N1-C2	5.03	121.78	115.88
3	B	403	GDP	C6-N1-C2	5.23	122.01	115.88
3	D	403	GDP	C6-N1-C2	5.70	122.56	115.88
3	C	1002	GDP	C6-N1-C2	5.72	122.59	115.88

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 ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	351/364 (96%)	-0.58	2 (0%) 90 91	10, 18, 31, 49	0
1	B	351/364 (96%)	-0.55	3 (0%) 85 87	11, 18, 32, 46	0
1	C	355/364 (97%)	-0.51	1 (0%) 94 94	11, 19, 35, 46	0
1	D	351/364 (96%)	-0.52	2 (0%) 90 91	11, 18, 32, 45	0
All	All	1408/1456 (96%)	-0.54	8 (0%) 90 91	10, 18, 33, 49	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	GLY	6.9
1	D	22	GLY	4.2
1	B	348	ARG	3.0
1	B	22	GLY	2.9
1	A	368	THR	2.7
1	B	368	THR	2.3
1	D	348	ARG	2.3
1	C	301	LYS	2.2

### 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

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
5	GOL	A	1004	6/6	0.81	0.13	0.62	34,39,42,48	0
3	GDP	C	1002	28/28	0.98	0.08	-0.16	11,16,19,20	0
2	NAP	D	402	48/48	0.98	0.06	-0.52	8,13,18,20	0
2	NAP	A	1001	48/48	0.98	0.06	-0.56	9,14,16,19	0
2	NAP	B	402	48/48	0.98	0.06	-0.68	9,13,15,16	0
4	GFB	B	401	38/38	0.98	0.06	-0.68	14,17,21,23	0
4	GFB	D	401	38/38	0.98	0.07	-0.72	13,19,24,24	0
2	NAP	C	1001	48/48	0.99	0.05	-0.85	8,12,15,16	0
4	GFB	C	1003	38/38	0.98	0.06	-0.87	14,19,23,24	0
4	GFB	A	1003	38/38	0.97	0.07	-0.90	15,20,26,27	0
3	GDP	B	403	28/28	0.98	0.06	-1.02	10,16,18,18	0
3	GDP	D	403	28/28	0.98	0.06	-1.38	12,15,20,22	0
3	GDP	A	1002	28/28	0.99	0.05	-1.80	11,14,19,23	0

## 6.5 Other polymers

There are no such residues in this entry.