



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:02 PM GMT

PDB ID : 1N7G  
Title : Crystal Structure of the GDP-mannose 4,6-dehydratase ternary complex with NADPH and GDP-rhamnose.  
Authors : Mulichak, A.M.; Bonin, C.P.; Reiter, W.-D.; Garavito, R.M.  
Deposited on : 2002-11-14  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (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

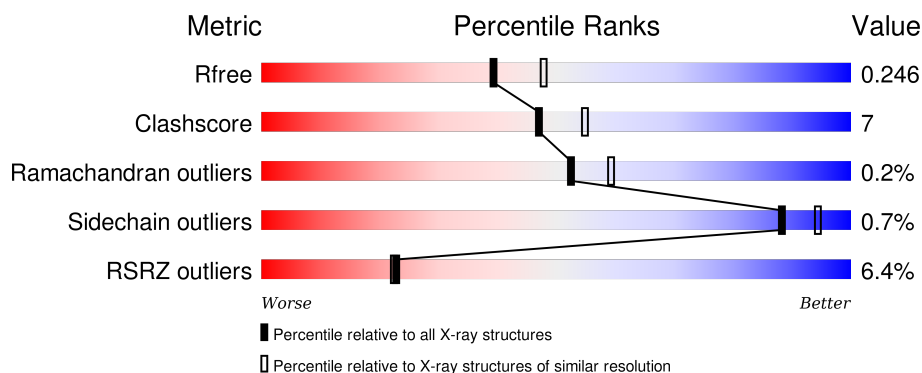
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	381	<div> <div>4%</div> <div>74% 13% 13%</div> </div>
1	B	381	<div> <div>4%</div> <div>70% 18% 12%</div> </div>
1	C	381	<div> <div>5%</div> <div>73% 14% 12%</div> </div>
1	D	381	<div> <div>8%</div> <div>71% 10% 18%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11034 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-D-mannose-4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2625	1675	453	488	9			
1	B	336	Total	C	N	O	S	0	0	0
			2626	1676	451	490	9			
1	C	334	Total	C	N	O	S	0	0	0
			2620	1672	449	490	9			
1	D	313	Total	C	N	O	S	0	0	0
			2382	1514	414	446	8			

There are 32 discrepancies between the modelled and reference sequences:

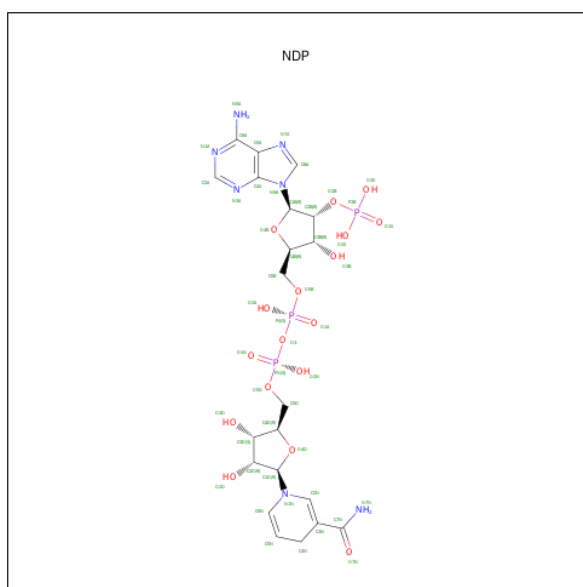
Chain	Residue	Modelled	Actual	Comment	Reference
A	374	LEU	-	EXPRESSION TAG	UNP P93031
A	375	GLU	-	EXPRESSION TAG	UNP P93031
A	376	HIS	-	EXPRESSION TAG	UNP P93031
A	377	HIS	-	EXPRESSION TAG	UNP P93031
A	378	HIS	-	EXPRESSION TAG	UNP P93031
A	379	HIS	-	EXPRESSION TAG	UNP P93031
A	380	HIS	-	EXPRESSION TAG	UNP P93031
A	381	HIS	-	EXPRESSION TAG	UNP P93031
B	374	LEU	-	EXPRESSION TAG	UNP P93031
B	375	GLU	-	EXPRESSION TAG	UNP P93031
B	376	HIS	-	EXPRESSION TAG	UNP P93031
B	377	HIS	-	EXPRESSION TAG	UNP P93031
B	378	HIS	-	EXPRESSION TAG	UNP P93031
B	379	HIS	-	EXPRESSION TAG	UNP P93031
B	380	HIS	-	EXPRESSION TAG	UNP P93031
B	381	HIS	-	EXPRESSION TAG	UNP P93031
C	374	LEU	-	EXPRESSION TAG	UNP P93031
C	375	GLU	-	EXPRESSION TAG	UNP P93031
C	376	HIS	-	EXPRESSION TAG	UNP P93031
C	377	HIS	-	EXPRESSION TAG	UNP P93031
C	378	HIS	-	EXPRESSION TAG	UNP P93031

*Continued on next page...*

Continued from previous page...

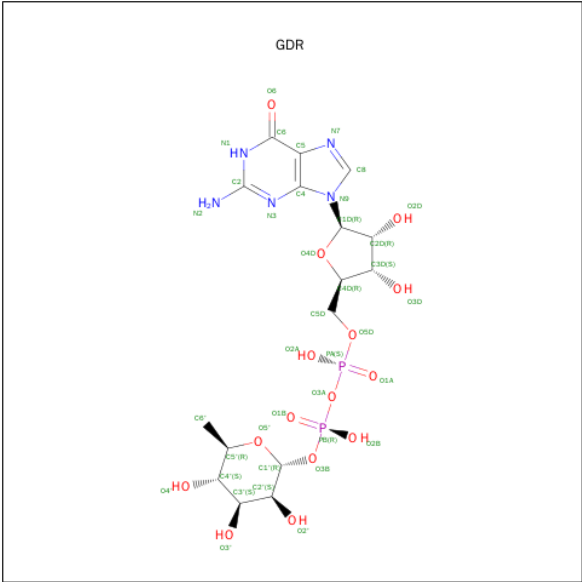
Chain	Residue	Modelled	Actual	Comment	Reference
C	379	HIS	-	EXPRESSION TAG	UNP P93031
C	380	HIS	-	EXPRESSION TAG	UNP P93031
C	381	HIS	-	EXPRESSION TAG	UNP P93031
D	374	LEU	-	EXPRESSION TAG	UNP P93031
D	375	GLU	-	EXPRESSION TAG	UNP P93031
D	376	HIS	-	EXPRESSION TAG	UNP P93031
D	377	HIS	-	EXPRESSION TAG	UNP P93031
D	378	HIS	-	EXPRESSION TAG	UNP P93031
D	379	HIS	-	EXPRESSION TAG	UNP P93031
D	380	HIS	-	EXPRESSION TAG	UNP P93031
D	381	HIS	-	EXPRESSION TAG	UNP P93031

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-RHAMNOSE (three-letter code: GDR) (formula:  $C_{16}H_{25}N_5O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	3	Total	C	N	O	P	0	0
			114	48	15	45	6		

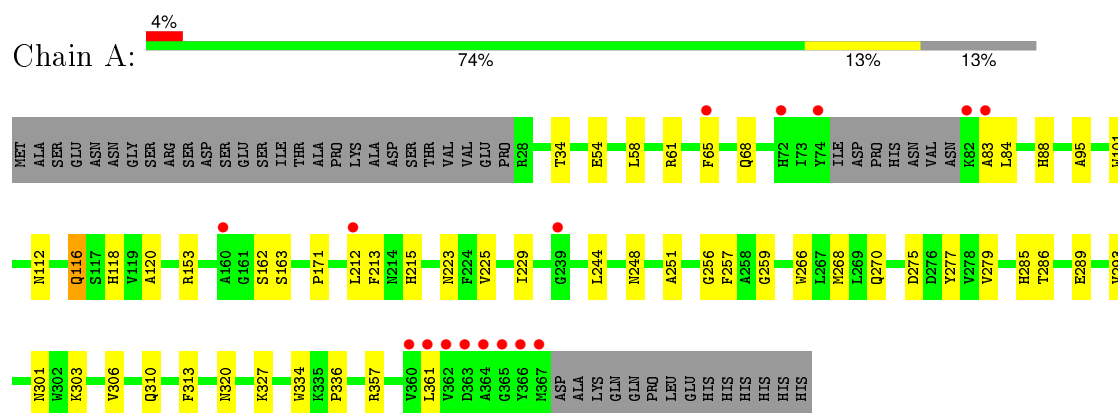
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	140	Total	O	0
			140	140	
4	B	109	Total	O	0
			109	109	
4	C	130	Total	O	0
			130	130	
4	D	96	Total	O	0
			96	96	

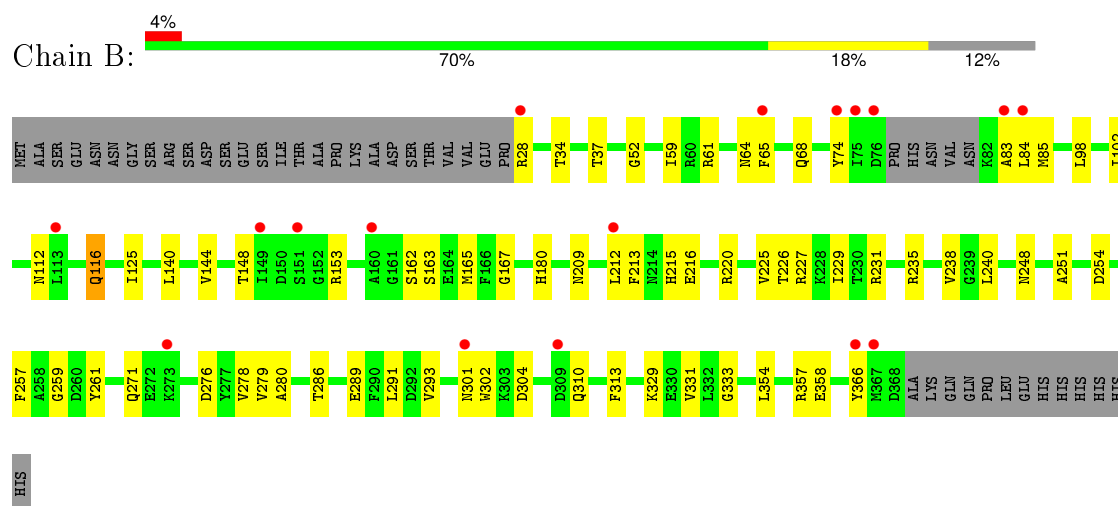
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

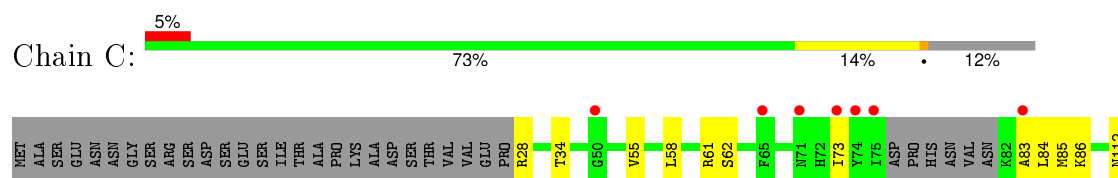
- Molecule 1: GDP-D-mannose-4,6-dehydratase

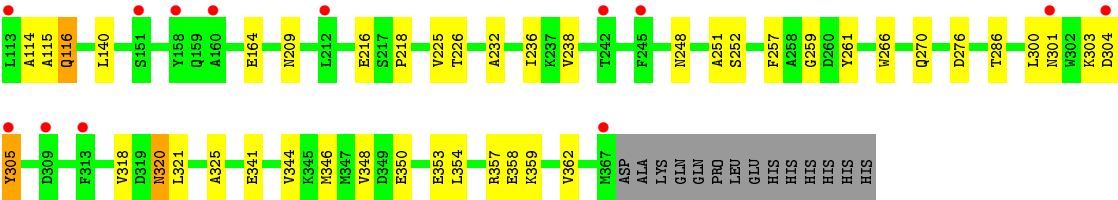


- Molecule 1: GDP-D-mannose-4,6-dehydratase

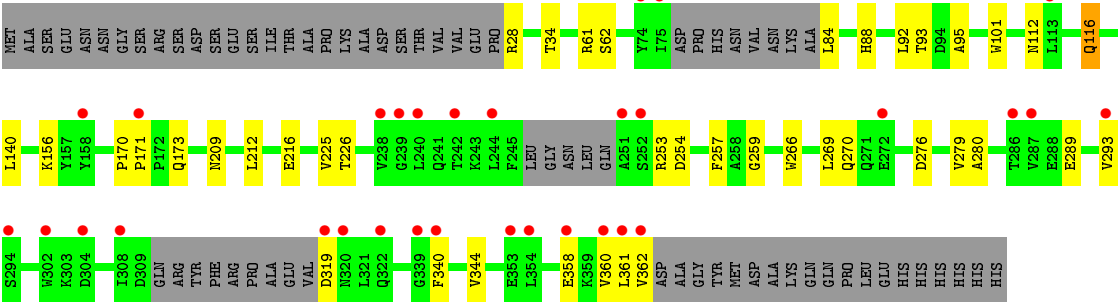


- Molecule 1: GDP-D-mannose-4,6-dehydratase





● Molecule 1: GDP-D-mannose-4,6-dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.18Å 119.01Å 118.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 28.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 87.8 (28.86-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.20Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.201 , 0.247 0.201 , 0.246	Depositor DCC
$R_{free}$ test set	3521 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 60.5	EDS
Estimated twinning fraction	0.013 for -h,l,k 0.015 for -k,-h,l 0.015 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 77293 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.44% 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: NDP, GDR

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	0.31	0/2688	0.57	2/3648 (0.1%)
1	B	0.30	0/2689	0.56	1/3653 (0.0%)
1	C	0.31	0/2683	0.56	1/3644 (0.0%)
1	D	0.30	0/2434	0.55	1/3306 (0.0%)
All	All	0.30	0/10494	0.56	5/14251 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLN	N-CA-C	-6.80	92.64	111.00
1	B	116	GLN	N-CA-C	-6.69	92.93	111.00
1	D	116	GLN	N-CA-C	-6.32	93.95	111.00
1	C	116	GLN	N-CA-C	-6.26	94.09	111.00
1	A	54	GLU	N-CA-C	-5.35	96.54	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2625	0	2532	33	0
1	B	2626	0	2510	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2620	0	2510	35	0
1	D	2382	0	2239	26	0
2	A	48	0	26	4	0
2	B	48	0	26	6	0
2	C	48	0	26	5	0
2	D	48	0	26	1	0
3	A	114	0	69	17	0
4	A	140	0	0	4	0
4	B	109	0	0	0	0
4	C	130	0	0	3	0
4	D	96	0	0	2	0
All	All	11034	0	9964	153	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 7.

The worst 5 of 153 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)
2:A:701:NDP:H41N	3:A:801:GDR:HC62	1.41	1.02
3:A:802:GDR:HC62	2:B:702:NDP:H41N	1.44	0.97
3:A:803:GDR:HC62	2:C:703:NDP:H41N	1.52	0.90
1:B:231:ARG:HG3	1:B:235:ARG:HH12	1.46	0.80
1:B:215:HIS:CE1	2:B:702:NDP:H42N	2.17	0.79

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	329/381 (86%)	319 (97%)	9 (3%)	1 (0%)	46 50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	332/381 (87%)	325 (98%)	6 (2%)	1 (0%)	46	50
1	C	330/381 (87%)	318 (96%)	12 (4%)	0	100	100
1	D	305/381 (80%)	295 (97%)	10 (3%)	0	100	100
All	All	1296/1524 (85%)	1257 (97%)	37 (3%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ALA
1	B	83	ALA

### 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	270/323 (84%)	269 (100%)	1 (0%)	93	97
1	B	267/323 (83%)	266 (100%)	1 (0%)	93	97
1	C	268/323 (83%)	264 (98%)	4 (2%)	72	84
1	D	235/323 (73%)	234 (100%)	1 (0%)	93	97
All	All	1040/1292 (80%)	1033 (99%)	7 (1%)	88	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	305	TYR
1	D	116	GLN
1	C	320	ASN
1	B	116	GLN
1	C	354	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	248	ASN
1	C	320	ASN
1	D	173	GLN
1	C	223	ASN
1	D	180	HIS

### 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](#)

7 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	NDP	A	701	-	42,52,52	1.12	2 (4%)	55,80,80	0.80	1 (1%)
3	GDR	A	801	-	33,41,41	0.96	2 (6%)	46,64,64	1.80	3 (6%)
3	GDR	A	802	-	33,41,41	1.00	2 (6%)	46,64,64	1.81	3 (6%)
3	GDR	A	803	-	33,41,41	0.98	2 (6%)	46,64,64	1.82	3 (6%)
2	NDP	B	702	-	42,52,52	1.16	2 (4%)	55,80,80	0.83	3 (5%)
2	NDP	C	703	-	42,52,52	1.14	2 (4%)	55,80,80	0.84	3 (5%)
2	NDP	D	704	-	42,52,52	1.16	2 (4%)	55,80,80	0.86	3 (5%)

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	NDP	A	701	-	-	0/30/77/77	0/5/5/5
3	GDR	A	801	-	-	0/17/57/57	0/4/4/4
3	GDR	A	802	-	-	0/17/57/57	0/4/4/4
3	GDR	A	803	-	-	0/17/57/57	0/4/4/4
2	NDP	B	702	-	-	0/30/77/77	0/5/5/5
2	NDP	C	703	-	-	0/30/77/77	0/5/5/5
2	NDP	D	704	-	-	0/30/77/77	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	NDP	C4N-C5N	-5.37	1.37	1.49
2	B	702	NDP	C4N-C5N	-5.34	1.37	1.49
2	C	703	NDP	C4N-C5N	-5.27	1.37	1.49
2	A	701	NDP	C4N-C5N	-5.12	1.38	1.49
2	D	704	NDP	P2B-O2B	-3.30	1.50	1.60

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	GDR	C5-C6-N1	-8.85	111.48	123.59
3	A	802	GDR	C5-C6-N1	-8.81	111.54	123.59
3	A	801	GDR	C5-C6-N1	-8.79	111.57	123.59
2	D	704	NDP	O4B-C1B-C2B	-2.66	101.78	106.60
2	B	702	NDP	O4B-C1B-C2B	-2.39	102.28	106.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NDP	4	0
3	A	801	GDR	7	0
3	A	802	GDR	4	0
3	A	803	GDR	6	0
2	B	702	NDP	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	NDP	5	0
2	D	704	NDP	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 [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	333/381 (87%)	0.03	16 (4%) 34 34	20, 32, 46, 60	0
1	B	336/381 (88%)	0.17	17 (5%) 32 31	22, 35, 48, 61	0
1	C	334/381 (87%)	0.26	20 (5%) 25 25	20, 36, 47, 54	0
1	D	313/381 (82%)	0.35	31 (9%) 9 8	23, 35, 54, 59	0
All	All	1316/1524 (86%)	0.20	84 (6%) 23 22	20, 34, 50, 61	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	ALA	6.4
1	D	361	LEU	5.6
1	D	74	TYR	4.5
1	B	83	ALA	4.4
1	C	74	TYR	4.3

### 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
2	NDP	A	701	48/48	0.97	0.13	-0.38	20,24,29,30	0
2	NDP	C	703	48/48	0.96	0.14	-0.40	21,27,36,38	0
3	GDR	A	803	38/38	0.94	0.13	-0.49	38,43,47,47	0
2	NDP	D	704	48/48	0.97	0.12	-0.51	23,28,34,35	0
2	NDP	B	702	48/48	0.98	0.13	-0.52	23,26,36,37	0
3	GDR	A	801	38/38	0.95	0.13	-0.58	34,38,40,41	0
3	GDR	A	802	38/38	0.93	0.12	-0.62	40,43,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.