



# wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 10:13 AM GMT

PDB ID : 3HN3  
Title : Human beta-glucuronidase at 1.7 Å resolution  
Authors : Klei, H.E.; Ghosh, K.; Anumula, R.  
Deposited on : 2009-05-29  
Resolution : 1.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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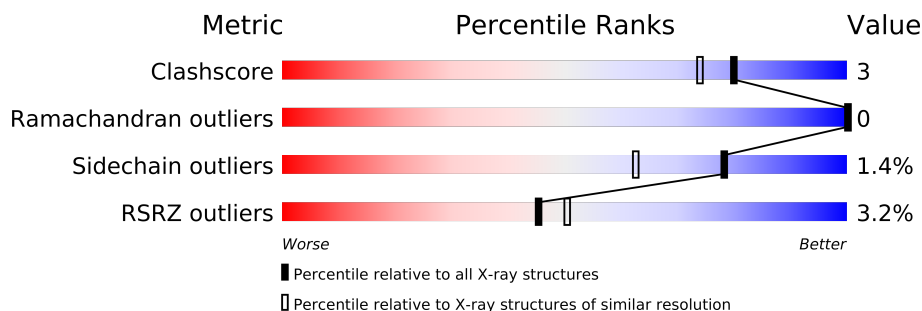
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	613	
1	B	613	
1	D	613	
1	E	613	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MRD	A	1	-	X
4	MRD	D	3	-	X
5	NAG	B	650	-	X
5	NAG	D	650	-	X
5	NAG	E	650	-	X
7	MPD	B	2	-	X
7	MPD	E	4	-	X

## 2 Entry composition i

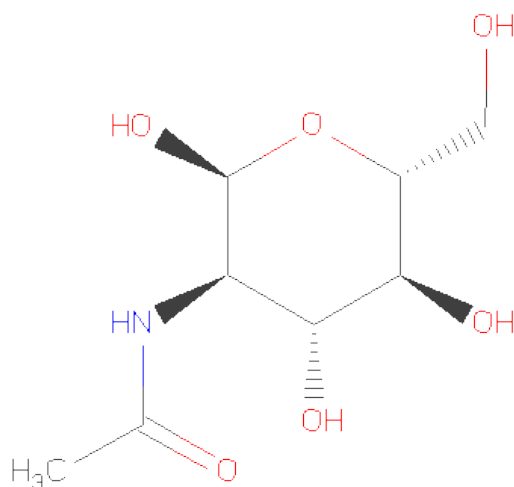
There are 10 unique types of molecules in this entry. The entry contains 23390 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	7	10	0
			5014	3227	855	917	15			
1	B	609	Total	C	N	O	S	10	8	0
			5007	3225	847	920	15			
1	D	607	Total	C	N	O	S	4	10	0
			5013	3223	856	918	16			
1	E	606	Total	C	N	O	S	10	7	0
			4977	3208	844	910	15			

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

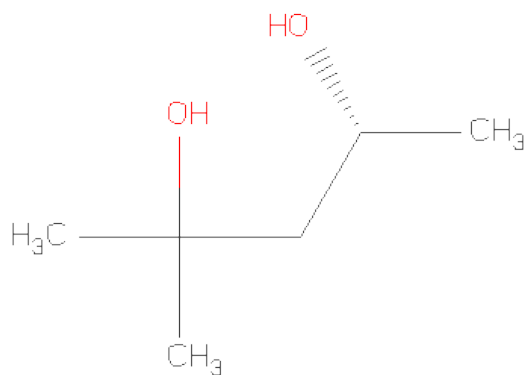


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

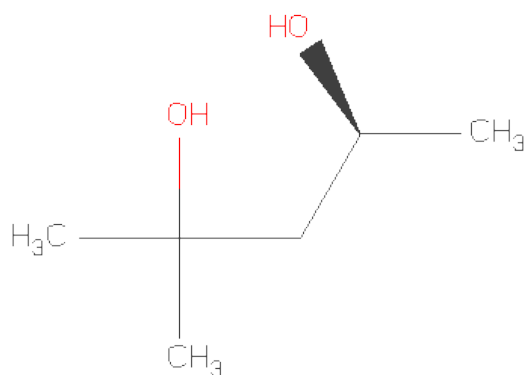


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

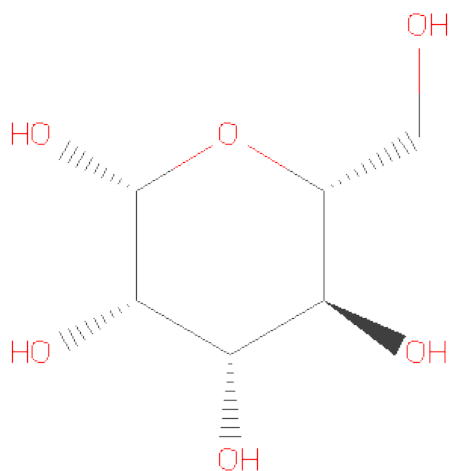


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		
7	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	10	Total	C	N	O	0	0
			116	64	2	50		
8	E	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 9 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			12	6	6		

- Molecule 10 is water.

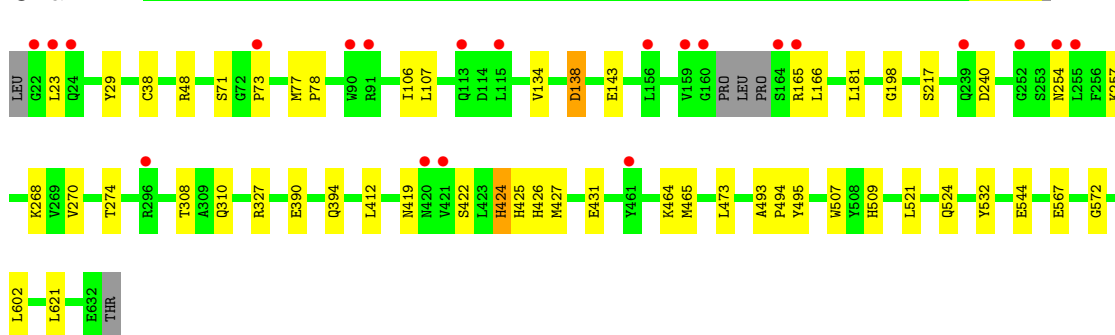
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	691	Total	O	0	0
			691	691		
10	B	706	Total	O	0	0
			706	706		
10	D	646	Total	O	0	0
			646	646		
10	E	764	Total	O	0	0
			764	764		

### 3 Residue-property plots

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.

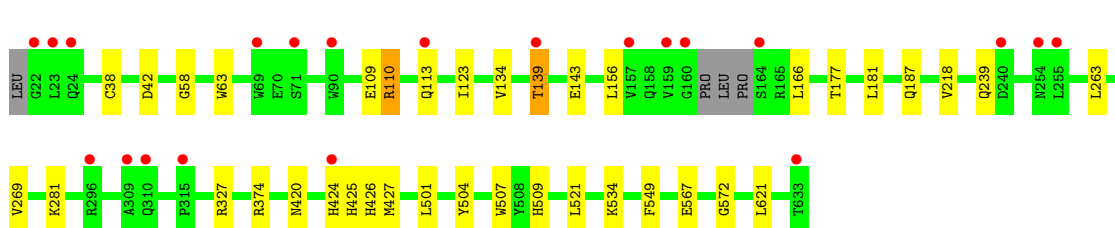
- Molecule 1: Beta-glucuronidase

Chain A:



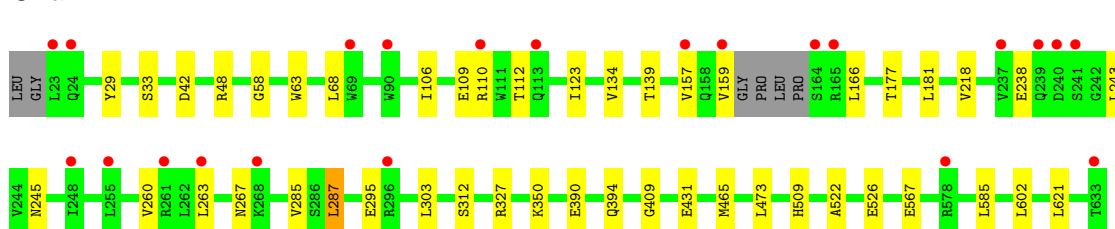
- Molecule 1: Beta-glucuronidase

Chain B:



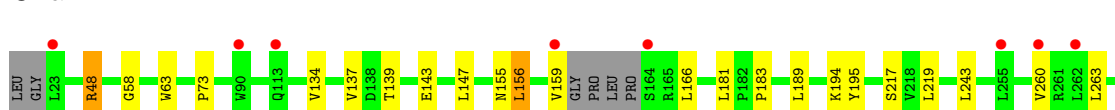
- Molecule 1: Beta-glucuronidase

Chain D:



- Molecule 1: Beta-glucuronidase

Chain E:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.58Å 123.11Å 266.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.70 19.92 – 1.66	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.90-1.70) 84.5 (19.92-1.66)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.240 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 315926 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8970e-04.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, NDG, GUP, MRD, MAN

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	0.48	2/5203 (0.0%)	0.63	1/7080 (0.0%)
1	B	0.49	4/5188 (0.1%)	0.65	3/7063 (0.0%)
1	D	0.44	0/5199	0.63	1/7076 (0.0%)
1	E	0.70	5/5150 (0.1%)	0.66	5/7012 (0.1%)
All	All	0.54	11/20740 (0.1%)	0.64	10/28231 (0.0%)

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	E	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	266	GLU	CD-OE1	27.08	1.55	1.25
1	E	266	GLU	CD-OE2	-23.65	0.99	1.25
1	E	194	LYS	CD-CE	-12.30	1.20	1.51
1	A	424	HIS	CB-CG	-11.31	1.29	1.50
1	B	239	GLN	CD-OE1	-9.06	1.04	1.24

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ARG	CB-CG-CD	10.21	138.13	111.60
1	E	295	GLU	OE1-CD-OE2	-10.02	111.28	123.30
1	E	194	LYS	CG-CD-CE	8.36	136.97	111.90
1	E	266	GLU	CG-CD-OE2	7.32	132.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	HIS	CA-CB-CG	5.85	123.54	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	295	GLU	Sidechain

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5014	0	4876	36	0
1	B	5007	0	4864	28	0
1	D	5013	0	4860	34	0
1	E	4977	0	4833	37	0
2	A	14	0	13	2	0
3	A	116	0	97	1	0
4	A	8	0	14	1	0
4	D	8	0	14	3	0
4	E	8	0	14	0	0
5	B	14	0	13	0	0
5	D	14	0	13	1	0
5	E	14	0	13	0	0
6	B	116	0	97	0	0
7	B	8	0	14	1	0
7	E	8	0	14	1	0
8	D	116	0	97	1	0
8	E	116	0	97	3	0
9	E	12	0	12	3	0
10	A	691	0	0	7	0
10	B	706	0	0	5	0
10	D	646	0	0	7	0
10	E	764	0	0	5	0
All	All	23390	0	19955	138	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 138 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:465:MET:HA	1:D:465:MET:HE2	1.52	0.90
1:D:390[B]:GLU:OE1	10:D:2481:HOH:O	1.91	0.86
1:E:183:PRO:HG3	1:E:412:LEU:HD23	1.57	0.86
1:B:143[B]:GLU:OE1	1:B:425:HIS:NE2	2.10	0.85
1:E:134:VAL:HG13	1:E:166:LEU:HD11	1.65	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	614/613 (100%)	592 (96%)	22 (4%)	0	100	100
1	B	614/613 (100%)	593 (97%)	21 (3%)	0	100	100
1	D	613/613 (100%)	594 (97%)	19 (3%)	0	100	100
1	E	609/613 (99%)	586 (96%)	23 (4%)	0	100	100
All	All	2450/2452 (100%)	2365 (96%)	85 (4%)	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	547/542 (101%)	538 (98%)	9 (2%)	75	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	546/542 (101%)	540 (99%)	6 (1%)	84	72
1	D	548/542 (101%)	542 (99%)	6 (1%)	84	72
1	E	542/542 (100%)	533 (98%)	9 (2%)	73	55
All	All	2183/2168 (101%)	2153 (99%)	30 (1%)	78	62

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	509	HIS
1	D	110	ARG
1	E	327	ARG
1	D	109	GLU
1	D	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	279	GLN
1	B	575	GLN
1	D	245	ASN
1	D	279	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

40 carbohydrates 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	$\# Z  > 2$
3	NAG	A	651	1,3	12,14,15	0.60	0	15,19,21	0.93	0
3	NAG	A	652	3	12,14,15	0.66	0	15,19,21	1.24	2 (13%)
3	BMA	A	653	3	10,11,12	0.58	0	11,15,17	0.94	1 (9%)
3	MAN	A	654	3	10,11,12	0.83	1 (10%)	11,15,17	0.87	0
3	MAN	A	655	3	10,11,12	0.72	0	11,15,17	1.09	1 (9%)
3	MAN	A	656	3	10,11,12	0.73	0	11,15,17	0.65	0
3	MAN	A	657	3	10,11,12	0.72	0	11,15,17	0.98	1 (9%)
3	GUP	A	658	3	10,11,12	0.71	0	11,15,17	0.72	0
3	MAN	A	659	3	10,11,12	0.78	1 (10%)	11,15,17	0.95	0
3	MAN	A	660	3	10,11,12	0.77	1 (10%)	11,15,17	0.50	0
6	NAG	B	651	1,6	12,14,15	0.62	0	15,19,21	0.77	0
6	NAG	B	652	6	12,14,15	0.79	1 (8%)	15,19,21	1.30	1 (6%)
6	BMA	B	653	6	10,11,12	0.57	0	11,15,17	1.02	0
6	MAN	B	654	6	10,11,12	0.69	0	11,15,17	0.96	0
6	MAN	B	655	6	10,11,12	0.74	0	11,15,17	1.11	1 (9%)
6	MAN	B	656	6	10,11,12	0.85	0	11,15,17	0.75	0
6	BMA	B	657	6	10,11,12	0.98	1 (10%)	11,15,17	1.32	2 (18%)
6	MAN	B	658	6	10,11,12	0.67	0	11,15,17	0.93	1 (9%)
6	MAN	B	659	6	10,11,12	0.75	0	11,15,17	0.77	0
6	MAN	B	660	6	10,11,12	0.87	1 (10%)	11,15,17	0.82	0
8	NAG	D	651	1,8	12,14,15	0.52	0	15,19,21	0.99	0
8	NAG	D	652	8	12,14,15	0.75	1 (8%)	15,19,21	1.24	2 (13%)
8	BMA	D	653	8	10,11,12	0.43	0	11,15,17	1.24	1 (9%)
8	MAN	D	654	8	10,11,12	0.62	0	11,15,17	1.03	0
8	MAN	D	655	8	10,11,12	0.72	0	11,15,17	0.86	1 (9%)
8	MAN	D	656	8	10,11,12	0.81	1 (10%)	11,15,17	0.70	0
8	MAN	D	657	8	10,11,12	0.80	0	11,15,17	1.64	3 (27%)
8	MAN	D	658	8	10,11,12	0.70	0	11,15,17	1.31	2 (18%)
8	MAN	D	659	8	10,11,12	0.74	0	11,15,17	0.67	0
8	MAN	D	660	8	10,11,12	0.81	0	11,15,17	0.84	0
8	NAG	E	651	1,8	12,14,15	0.73	0	15,19,21	0.76	0
8	NAG	E	652	8	12,14,15	0.54	0	15,19,21	1.55	2 (13%)
8	BMA	E	653	8	10,11,12	0.43	0	11,15,17	0.98	0
8	MAN	E	654	8	10,11,12	0.89	1 (10%)	11,15,17	1.09	0
8	MAN	E	655	8	10,11,12	0.59	0	11,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	E	656	8	10,11,12	0.75	0	11,15,17	0.85	0
8	MAN	E	657	8	10,11,12	0.75	0	11,15,17	0.84	0
8	MAN	E	658	8	10,11,12	0.60	0	11,15,17	1.38	3 (27%)
8	MAN	E	659	8	10,11,12	0.79	0	11,15,17	1.07	0
8	MAN	E	660	8	10,11,12	0.62	0	11,15,17	0.92	0

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	NAG	A	651	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	652	3	-	0/6/23/26	0/1/1/1
3	BMA	A	653	3	-	0/2/19/22	0/1/1/1
3	MAN	A	654	3	-	0/2/19/22	0/1/1/1
3	MAN	A	655	3	-	0/2/19/22	0/1/1/1
3	MAN	A	656	3	-	0/2/19/22	0/1/1/1
3	MAN	A	657	3	-	0/2/19/22	0/1/1/1
3	GUP	A	658	3	-	0/2/19/22	1/1/1/1
3	MAN	A	659	3	-	0/2/19/22	0/1/1/1
3	MAN	A	660	3	-	0/2/19/22	0/1/1/1
6	NAG	B	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	652	6	-	0/6/23/26	0/1/1/1
6	BMA	B	653	6	-	0/2/19/22	0/1/1/1
6	MAN	B	654	6	-	0/2/19/22	0/1/1/1
6	MAN	B	655	6	-	0/2/19/22	0/1/1/1
6	MAN	B	656	6	-	0/2/19/22	0/1/1/1
6	BMA	B	657	6	-	0/2/19/22	0/1/1/1
6	MAN	B	658	6	-	0/2/19/22	0/1/1/1
6	MAN	B	659	6	-	0/2/19/22	0/1/1/1
6	MAN	B	660	6	-	0/2/19/22	0/1/1/1
8	NAG	D	651	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	652	8	-	0/6/23/26	0/1/1/1
8	BMA	D	653	8	-	0/2/19/22	0/1/1/1
8	MAN	D	654	8	-	0/2/19/22	0/1/1/1
8	MAN	D	655	8	-	0/2/19/22	0/1/1/1
8	MAN	D	656	8	-	0/2/19/22	0/1/1/1
8	MAN	D	657	8	-	0/2/19/22	0/1/1/1
8	MAN	D	658	8	-	0/2/19/22	0/1/1/1
8	MAN	D	659	8	-	0/2/19/22	0/1/1/1
8	MAN	D	660	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	651	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	652	8	-	0/6/23/26	0/1/1/1
8	BMA	E	653	8	-	0/2/19/22	0/1/1/1
8	MAN	E	654	8	-	0/2/19/22	0/1/1/1
8	MAN	E	655	8	-	0/2/19/22	0/1/1/1
8	MAN	E	656	8	-	0/2/19/22	0/1/1/1
8	MAN	E	657	8	-	0/2/19/22	0/1/1/1
8	MAN	E	658	8	-	0/2/19/22	0/1/1/1
8	MAN	E	659	8	-	0/2/19/22	0/1/1/1
8	MAN	E	660	8	-	0/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	657	BMA	O5-C5	-2.69	1.40	1.45
8	E	654	MAN	O5-C5	-2.37	1.41	1.45
6	B	660	MAN	O5-C5	-2.18	1.41	1.45
3	A	654	MAN	O5-C5	-2.14	1.41	1.45
8	D	652	NAG	O5-C5	-2.07	1.41	1.45

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	652	NAG	C3-C2-N2	-4.22	105.34	111.76
8	D	657	MAN	C4-C3-C2	3.53	115.24	110.50
8	D	658	MAN	O5-C5-C6	3.11	110.25	106.98
6	B	652	NAG	C3-C2-N2	-3.06	107.10	111.76
8	D	657	MAN	C3-C4-C5	2.83	115.25	110.20

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	658	GUP	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry ⓘ

10 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$
4	MRD	A	1	-	7,7,7	0.27	0	10,10,10	0.42	0
2	NDG	A	650	1	12,14,15	0.47	0	15,19,21	1.59	3 (20%)
7	MPD	B	2	-	7,7,7	0.33	0	10,10,10	0.67	0
5	NAG	B	650	1	12,14,15	0.75	1 (8%)	15,19,21	0.77	0
4	MRD	D	3	-	7,7,7	0.28	0	10,10,10	0.67	0
5	NAG	D	650	1	12,14,15	0.64	0	15,19,21	0.85	0
7	MPD	E	4	-	7,7,7	0.23	0	10,10,10	0.46	0
4	MRD	E	5	-	7,7,7	0.25	0	10,10,10	0.22	0
5	NAG	E	650	1	12,14,15	0.63	0	15,19,21	0.86	0
9	BMA	E	661	-	12,12,12	0.57	0	17,17,17	2.05	4 (23%)

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	MRD	A	1	-	-	0/5/5/5	0/0/0/0
2	NDG	A	650	1	-	0/6/23/26	0/1/1/1
7	MPD	B	2	-	-	0/5/5/5	0/0/0/0
5	NAG	B	650	1	-	0/6/23/26	0/1/1/1
4	MRD	D	3	-	-	0/5/5/5	0/0/0/0
5	NAG	D	650	1	-	0/6/23/26	0/1/1/1
7	MPD	E	4	-	-	0/5/5/5	0/0/0/0
4	MRD	E	5	-	-	0/5/5/5	0/0/0/0
5	NAG	E	650	1	-	0/6/23/26	0/1/1/1
9	BMA	E	661	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	650	NAG	O5-C5	-2.15	1.41	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	661	BMA	O5-C1-C2	5.11	117.78	109.86
9	E	661	BMA	C1-O5-C5	4.39	121.26	113.40
2	A	650	NDG	O-C5-C6	4.05	111.23	106.98
2	A	650	NDG	C3-C2-N2	-2.77	107.54	111.76
9	E	661	BMA	C3-C4-C5	-2.75	105.30	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	608/613 (99%)	0.30	21 (3%)	42 47	6, 13, 27, 36	2 (0%)
1	B	609/613 (99%)	0.23	21 (3%)	43 48	5, 12, 24, 34	3 (0%)
1	D	607/613 (99%)	0.24	22 (3%)	41 46	6, 13, 27, 33	1 (0%)
1	E	606/613 (98%)	0.20	16 (2%)	53 58	6, 12, 23, 30	6 (0%)
All	All	2430/2452 (99%)	0.24	80 (3%)	45 49	5, 12, 26, 36	12 (0%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	LEU	7.6
1	A	159	VAL	7.5
1	D	23	LEU	7.1
1	B	160	GLY	6.8
1	D	633	THR	6.3

### 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 ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	A	655	11/12	0.18	3.52	20,21,23,26	0
8	MAN	E	660	11/12	0.13	2.10	15,16,18,19	0
3	MAN	A	660	11/12	0.23	1.98	26,28,29,31	0
3	MAN	A	657	11/12	0.16	1.82	22,23,26,29	0
8	NAG	D	652	14/15	0.11	1.60	12,14,17,21	0
8	MAN	D	655	11/12	0.11	1.52	24,26,29,29	0
6	NAG	B	651	14/15	0.11	1.14	11,13,19,19	0
8	MAN	D	659	11/12	0.19	0.77	31,32,34,34	0
8	MAN	D	656	11/12	0.15	0.64	29,32,34,36	0
6	BMA	B	657	11/12	0.17	0.54	34,36,37,37	0
8	MAN	D	658	11/12	0.15	0.47	27,28,29,29	0
6	NAG	B	652	14/15	0.12	0.30	11,13,18,19	0
8	MAN	E	657	11/12	0.11	0.29	15,18,20,20	0
6	MAN	B	655	11/12	0.14	0.20	28,31,33,34	0
6	MAN	B	656	11/12	0.13	-0.02	23,27,30,30	0
8	NAG	E	652	14/15	0.09	-0.05	7,9,13,13	0
8	NAG	D	651	14/15	0.09	-0.06	9,12,14,15	0
3	MAN	A	659	11/12	0.11	-0.24	22,23,25,26	0
6	MAN	B	659	11/12	0.14	-0.29	26,26,28,29	0
8	MAN	E	658	11/12	0.08	-0.38	9,11,14,15	0
8	MAN	D	654	11/12	0.10	-0.44	19,21,23,24	0
3	NAG	A	651	14/15	0.09	-0.49	10,12,15,15	0
6	MAN	B	658	11/12	0.13	-0.49	18,20,21,23	0
8	MAN	E	659	11/12	0.08	-0.53	12,13,14,15	0
6	MAN	B	654	11/12	0.10	-0.64	15,17,20,23	0
8	NAG	E	651	14/15	0.07	-0.69	7,9,10,10	0
3	NAG	A	652	14/15	0.09	-1.11	12,14,18,19	0
3	BMA	A	653	11/12	0.10	-1.17	12,14,16,19	0
8	BMA	E	653	11/12	0.07	-1.21	7,9,10,11	0
6	BMA	B	653	11/12	0.09	-1.61	12,13,15,19	0
8	BMA	D	653	11/12	0.08	-1.97	13,16,18,23	0
8	MAN	E	656	11/12	0.08	-2.10	15,17,21,21	0
8	MAN	E	655	11/12	0.08	-2.25	11,14,16,17	0
3	MAN	A	654	11/12	0.09	-2.33	18,19,20,21	0
8	MAN	E	654	11/12	0.07	-5.06	8,11,13,14	0
3	MAN	A	656	11/12	0.18	-	28,30,32,33	0
3	GUP	A	658	11/12	0.31	-	34,36,38,39	0
8	MAN	D	657	11/12	0.35	-	40,42,43,44	0
8	MAN	D	660	11/12	0.17	-	32,34,36,36	0
6	MAN	B	660	11/12	0.21	-	37,40,41,41	0

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	D	650	14/15	0.24	6.65	31,33,35,36	0
5	NAG	E	650	14/15	0.18	3.27	24,30,34,34	0
4	MRD	D	3	8/8	0.15	2.66	25,27,29,30	0
4	MRD	A	1	8/8	0.17	2.38	23,26,27,28	0
7	MPD	E	4	8/8	0.17	2.36	24,26,28,29	0
5	NAG	B	650	14/15	0.14	2.31	20,22,24,25	0
7	MPD	B	2	8/8	0.13	2.24	20,23,25,27	0
2	NDG	A	650	14/15	0.21	1.98	37,40,41,41	0
4	MRD	E	5	8/8	0.20	1.85	36,36,37,38	0
9	BMA	E	661	12/12	0.21	-	33,36,36,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.