



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1GZE  
Title : STRUCTURE OF THE CLOSTRIDIUM BOTULINUM C3 EXOENZYME  
(L177C MUTANT)  
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Deposited on : 2002-05-21  
Resolution : 2.70 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.

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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

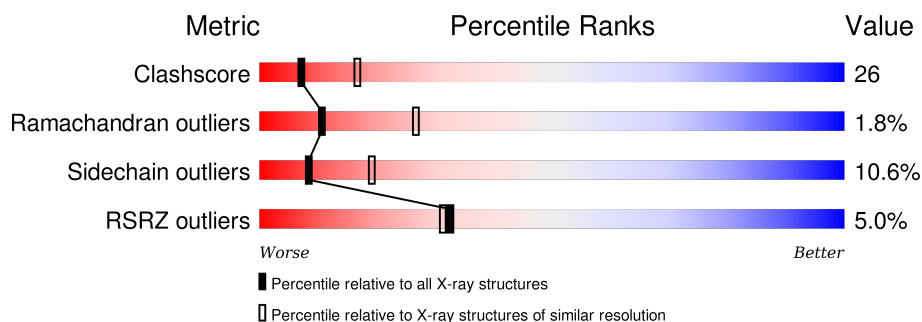
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	<div> <div>7%</div> <div>55%</div> <div>37%</div> <div>• • •</div> </div>
1	B	211	<div> <div>3%</div> <div>54%</div> <div>35%</div> <div>7%</div> <div>•</div> </div>
1	C	211	<div> <div>7%</div> <div>46%</div> <div>46%</div> <div>7%</div> </div>
1	D	211	<div> <div>3%</div> <div>56%</div> <div>35%</div> <div>5%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6511 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 MONO-ADP-RIBOSYLTRANSFERASE C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1623	1029	276	310	8			
1	B	203	Total	C	N	O	S	0	0	0
			1595	1011	272	304	8			
1	C	210	Total	C	N	O	S	0	0	0
			1651	1047	281	315	8			
1	D	203	Total	C	N	O	S	0	0	0
			1595	1011	272	304	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	CYS	LEU	ENGINEERED MUTATION	UNP P15879
B	177	CYS	LEU	ENGINEERED MUTATION	UNP P15879
C	177	CYS	LEU	ENGINEERED MUTATION	UNP P15879
D	177	CYS	LEU	ENGINEERED MUTATION	UNP P15879

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Hg	0	0
			1	1		
2	A	1	Total	Hg	0	0
			1	1		
2	D	1	Total	Hg	0	0
			1	1		
2	C	1	Total	Hg	0	0
			1	1		

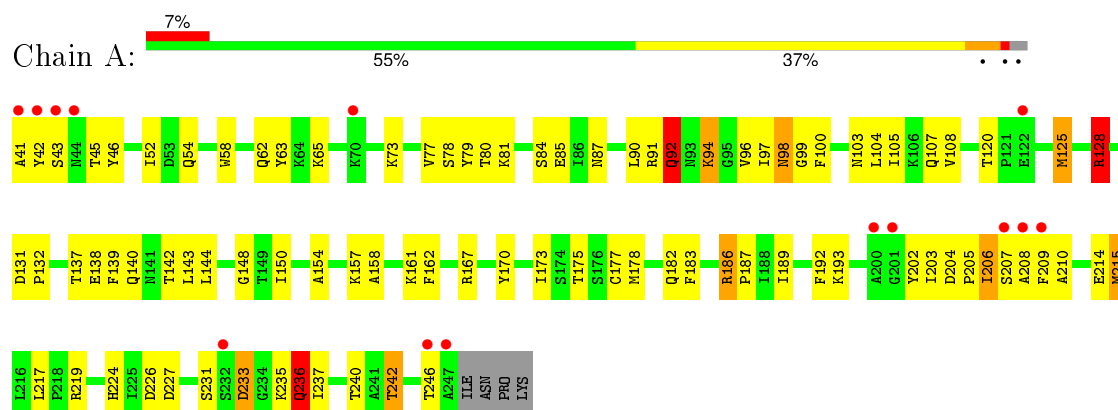
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	11	Total 11	O 11	0	0
3	C	11	Total 11	O 11	0	0
3	D	14	Total 14	O 14	0	0

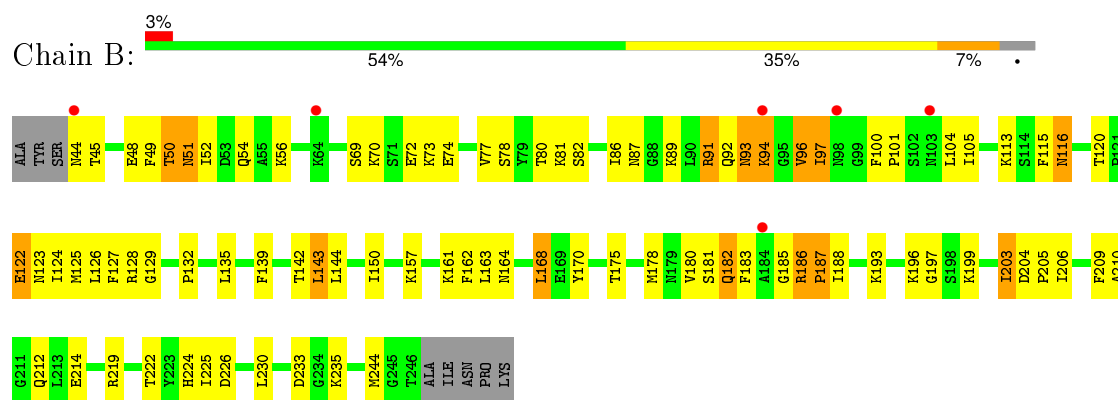
### 3 Residue-property plots

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

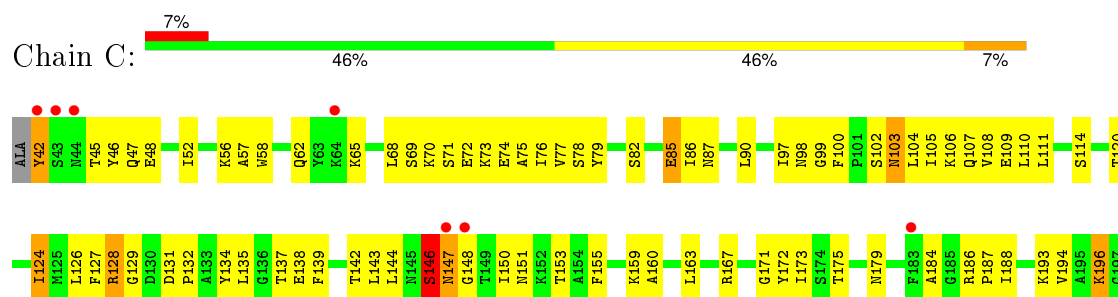
#### • Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3



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Residue	Score	Category
I225	0.00	Low
D226	0.00	Low
D227	0.00	Low
M228	0.00	Low
R229	0.00	Low
L230	0.00	Low
S231	0.00	Low
S232	0.00	Low
D233	0.00	Low
Q236	0.00	Low
I237	0.00	Low
I238	0.00	Low
I239	0.00	Low
M243	0.00	Low
Y244	0.00	Low
G245	0.00	Low
T246	0.00	Low
ALA	0.00	Low
ILE	0.00	Low
ASN	0.00	Low
PRO	0.00	Low
LYS	0.00	Low
E138	0.00	Low
F139	0.00	Low
L143	0.00	Low
L144	0.00	Low
N145	0.00	Low
S146	0.00	Low
N147	0.00	Low
G148	0.00	Low
T149	0.00	Low
I150	0.00	Low
N151	0.00	Low
K156	0.00	Low
K152	0.00	Low
F155	0.00	Low
E156	0.00	Low
K157	0.00	Low
A158	0.00	Low
K159	0.00	Low
F162	0.00	Low
L163	0.00	Low
N164	0.00	Low
K165	0.00	Low
D166	0.00	Low
R167	0.00	Low
Y172	0.00	Low
T175	0.00	Low
N179	0.00	Low
Q182	0.00	Low
F183	0.00	Low
G185	0.00	Low
R186	0.00	Low
F192	0.00	Low
K193	0.00	Low
K199	0.00	Low
A200	0.00	Low
G201	0.00	Low
D204	0.00	Low
P205	0.00	Low
I206	0.00	Low
S207	0.00	Low
A208	0.00	Low
F209	0.00	Low
E214	0.00	Low
M215	0.00	Low
L216	0.00	Low
Y223	0.00	Low
E224	0.00	Low
ALA	0.00	Low
TYR	0.00	Low
SER	0.00	Low
N44	0.00	Low
T45	0.00	Low
Y46	0.00	Low
N51	0.00	Low
I52	0.00	Low
D53	0.00	Low
Q54	0.00	Low
A55	0.00	Low
K56	0.00	Low
A57	0.00	Low
W58	0.00	Low
Q62	0.00	Low
Y66	0.00	Low
S69	0.00	Low
K70	0.00	Low
S71	0.00	Low
E72	0.00	Low
A75	0.00	Low
I76	0.00	Low
T80	0.00	Low
K89	0.00	Low
L90	0.00	Low
R91	0.00	Low
Q92	0.00	Low
I97	0.00	Low
N98	0.00	Low
G99	0.00	Low
F100	0.00	Low
P101	0.00	Low
S102	0.00	Low
N103	0.00	Low
L104	0.00	Low
I105	0.00	Low
V108	0.00	Low
L111	0.00	Low
F115	0.00	Low
P121	0.00	Low
L126	0.00	Low
F127	0.00	Low
R128	0.00	Low
G129	0.00	Low
D130	0.00	Low
Y132	0.00	Low

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.00Å 75.60Å 123.47Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	18.12 – 2.70 19.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.1 (18.12-2.70) 89.9 (19.85-2.71)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.240 , 0.290 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25841 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.78	3/1652 (0.2%)	1.55	10/2219 (0.5%)
1	B	0.64	0/1623	0.81	1/2179 (0.0%)
1	C	0.51	0/1681	0.76	2/2257 (0.1%)
1	D	0.57	0/1623	0.79	2/2179 (0.1%)
All	All	0.63	3/6579 (0.0%)	1.03	15/8834 (0.2%)

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	A	0	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	ARG	CD-NE	-10.92	1.27	1.46
1	A	186	ARG	NE-CZ	-9.54	1.20	1.33
1	A	186	ARG	CG-CD	5.38	1.65	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH1	36.97	138.78	120.30
1	A	186	ARG	NE-CZ-NH2	-33.10	103.75	120.30
1	A	186	ARG	CD-NE-CZ	31.86	168.20	123.60
1	A	186	ARG	CG-CD-NE	-8.71	93.51	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	PHE	N-CA-C	-8.14	89.01	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	B	187	PRO	Mainchain
1	B	96	VAL	Mainchain

## 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	1623	0	1633	84	0
1	B	1595	0	1609	84	0
1	C	1651	0	1665	95	0
1	D	1595	0	1609	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	0	0	0
3	B	11	0	0	1	0
3	C	11	0	0	0	0
3	D	14	0	0	0	0
All	All	6511	0	6516	339	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 26.

The worst 5 of 339 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:150:ILE:HD13	1:D:150:ILE:O	1.48	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LYS:HG3	1:C:251:LYS:O	1.52	1.07
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.23	1.02
1:D:70:LYS:N	1:D:70:LYS:HD3	1.77	0.99
1:C:251:LYS:CG	1:C:251:LYS:O	2.13	0.97

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	205/211 (97%)	175 (85%)	26 (13%)	4 (2%)	9	24
1	B	201/211 (95%)	181 (90%)	17 (8%)	3 (2%)	13	32
1	C	208/211 (99%)	175 (84%)	28 (14%)	5 (2%)	7	19
1	D	201/211 (95%)	173 (86%)	25 (12%)	3 (2%)	13	32
All	All	815/844 (97%)	704 (86%)	96 (12%)	15 (2%)	11	27

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	ASN
1	D	147	ASN
1	B	181	SER
1	D	66	TYR
1	A	65	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/179 (98%)	156 (89%)	19 (11%)	8	18
1	B	173/179 (97%)	158 (91%)	15 (9%)	13	29
1	C	179/179 (100%)	158 (88%)	21 (12%)	7	15
1	D	173/179 (97%)	154 (89%)	19 (11%)	8	18
All	All	700/716 (98%)	626 (89%)	74 (11%)	8	19

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	MET
1	C	111	LEU
1	D	157	LYS
1	C	42	TYR
1	C	71	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	HIS
1	C	87	ASN
1	D	140	GLN
1	C	47	GLN
1	C	54	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	207/211 (98%)	0.36	14 (6%) 20 19	38, 63, 86, 99	0
1	B	203/211 (96%)	0.10	6 (2%) 54 54	27, 58, 84, 91	0
1	C	210/211 (99%)	0.34	14 (6%) 21 19	39, 64, 89, 96	0
1	D	203/211 (96%)	0.06	7 (3%) 49 49	25, 52, 79, 91	0
All	All	823/844 (97%)	0.22	41 (4%) 32 31	25, 60, 86, 99	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	SER	7.9
1	A	41	ALA	7.7
1	C	42	TYR	6.8
1	A	42	TYR	6.7
1	A	43	SER	5.6

### 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	HG	A	1248	1/1	0.98	0.06	-2.73	62,62,62,62	0
2	HG	B	1247	1/1	0.98	0.11	-3.02	81,81,81,81	0
2	HG	D	1247	1/1	0.99	0.10	-	59,59,59,59	0
2	HG	C	1252	1/1	0.99	0.13	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.