



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:57 PM GMT

PDB ID : 4UDK  
Title : Crystal structure of b-1,4-mannopyranosyl-chitobiose phosphorylase at 1.76 Angstrom from unknown human gut bacteria (Uhgb\_MP) in complex with N-acetyl-D-glucosamine, beta-D-mannopyranose and inorganic phosphate  
Authors : Ladeveze, S.; Cioci, G.; Potocki-Veronese, G.; Tranier, S.; Mourey, L.  
Deposited on : 2014-12-10  
Resolution : 1.76 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

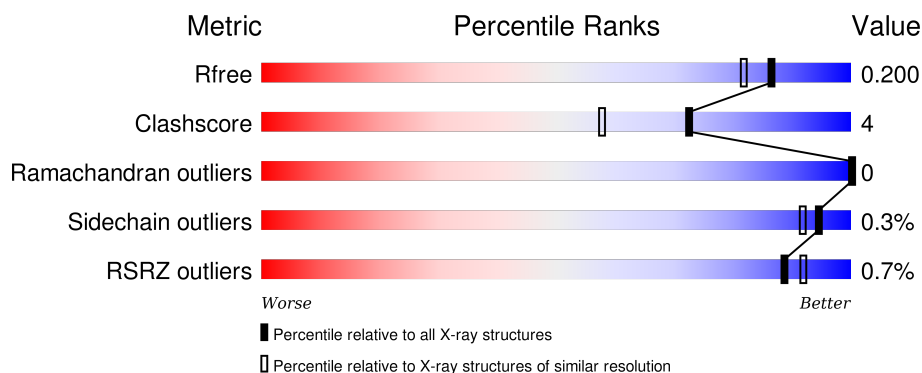
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	347	<div> <div>85%</div> <div>7% • 8%</div> </div>
1	B	347	<div> <div>82%</div> <div>10% 8%</div> </div>
1	C	347	<div> <div>84%</div> <div>7% • 8%</div> </div>
1	D	347	<div> <div>84%</div> <div>8% 8%</div> </div>
1	F	347	<div> <div>82%</div> <div>9% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	347	<div> <div></div> <div>%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	A	329	-	-	X	X
4	BMA	B	329	-	-	-	X
4	BMA	C	329	-	-	-	X
4	BMA	D	329	-	-	X	X
4	BMA	E	329	-	-	-	X
4	BMA	F	329	-	-	-	X
5	NDG	C	330	-	-	-	X
6	PGE	A	331	-	-	-	X
6	PGE	D	331	-	-	-	X
6	PGE	E	331	-	-	-	X
7	EDO	A	332	-	-	-	X
8	K	A	333	-	-	-	X
8	K	B	333	-	-	-	X
8	K	C	333	-	-	-	X
8	K	E	333	-	-	-	X
8	K	F	333	-	-	-	X
9	GOL	B	331	-	-	-	X
9	GOL	C	331	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17398 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 UHGB\_MP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	11	0
			2648	1710	445	476	17			
1	B	320	Total	C	N	O	S	0	15	0
			2686	1734	449	486	17			
1	C	319	Total	C	N	O	S	0	10	0
			2628	1699	437	475	17			
1	D	320	Total	C	N	O	S	0	14	0
			2679	1725	451	486	17			
1	F	320	Total	C	N	O	S	0	12	0
			2657	1713	447	480	17			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
A	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
A	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
A	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
A	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
A	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
B	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
B	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
B	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
B	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
B	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
C	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
C	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
C	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
C	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
C	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
D	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
D	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
D	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
D	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
F	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
F	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
F	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
F	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
F	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9

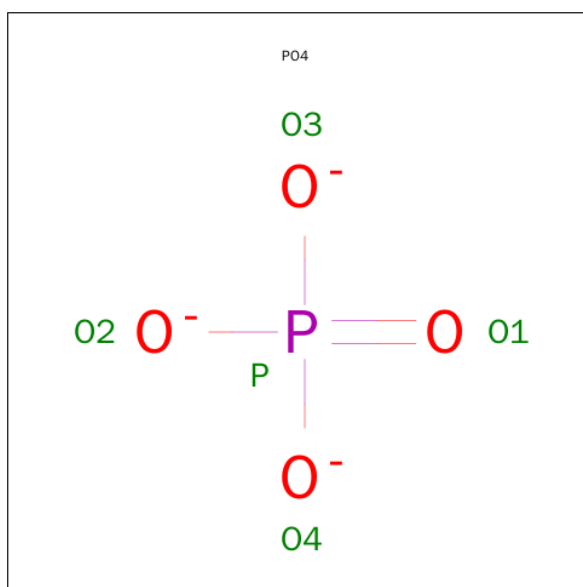
- Molecule 2 is a protein called UHGB\_MP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	321	Total	C	N	O	S	0	8	0
			2636	1701	441	477	17			

There are 21 discrepancies between the modelled and reference sequences:

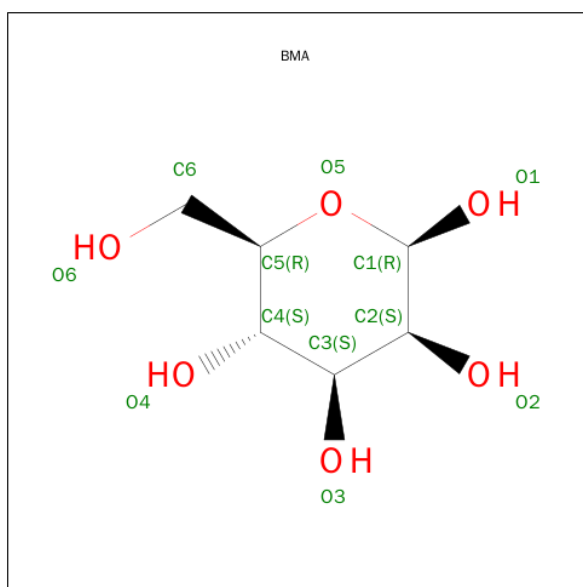
Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
E	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
E	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
E	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
E	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
E	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	7	ILE	VAL	CONFLICT	UNP D9ZDQ9

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



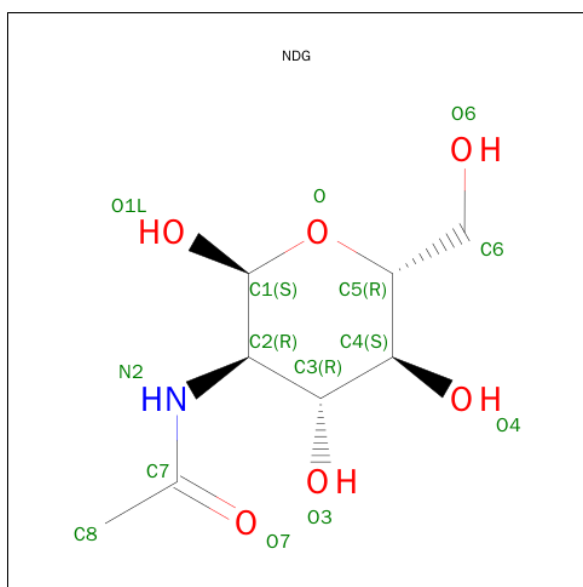
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



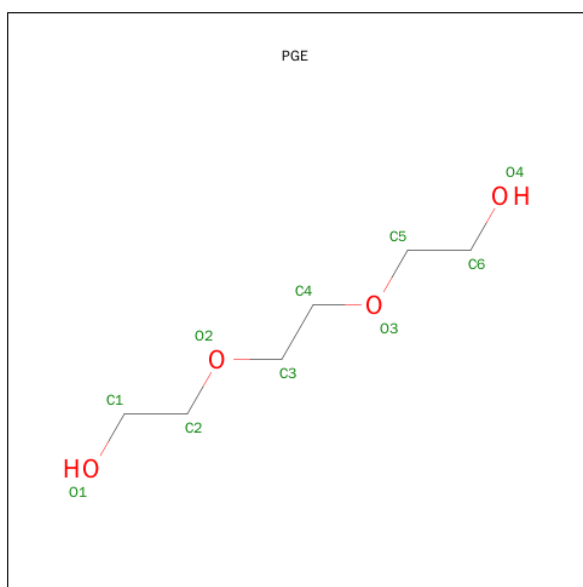
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		
4	E	1	Total	C	O	0	0
			12	6	6		
4	F	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 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>).



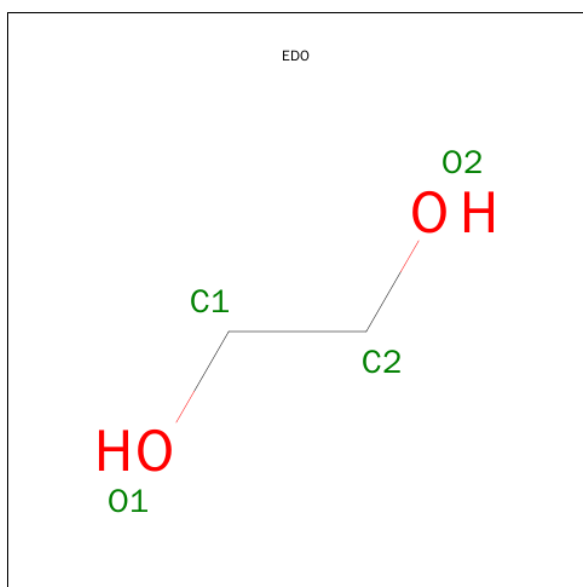
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	B	1	Total	C	N	O	0	0
			15	8	1	6		
5	C	1	Total	C	N	O	0	0
			15	8	1	6		
5	D	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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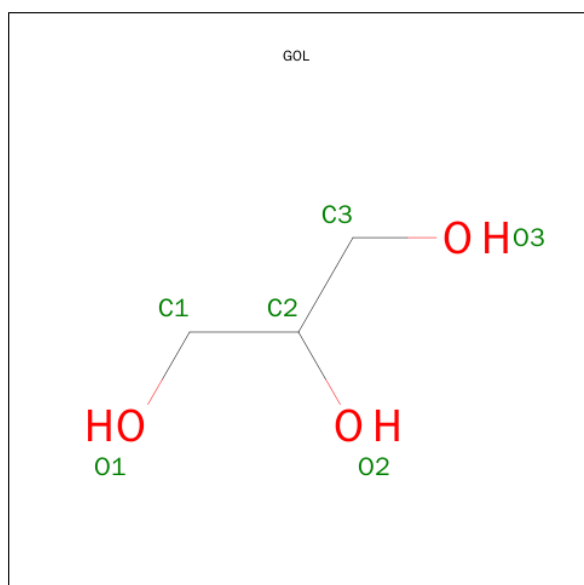
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	K	0	0
			1	1		
8	E	1	Total	K	0	0
			1	1		
8	B	1	Total	K	0	0
			1	1		
8	C	1	Total	K	0	0
			1	1		
8	A	1	Total	K	0	0
			1	1		
8	F	1	Total	K	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		

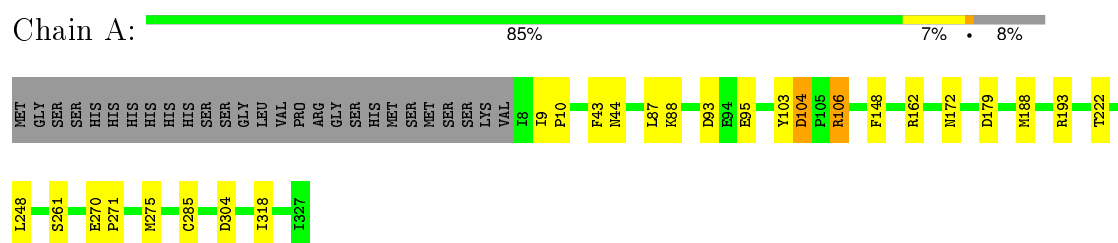
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	238	Total	O	0	0
			238	238		
10	B	226	Total	O	0	0
			226	226		
10	C	218	Total	O	0	0
			218	218		
10	D	181	Total	O	0	0
			181	181		
10	E	188	Total	O	0	0
			188	188		
10	F	153	Total	O	0	0
			153	153		

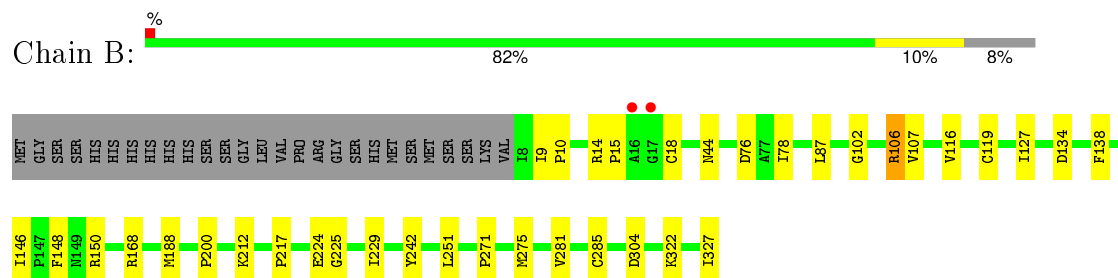
### 3 Residue-property plots [i](#)

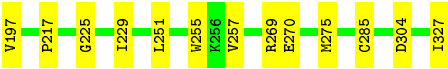
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: UHGB\_MP

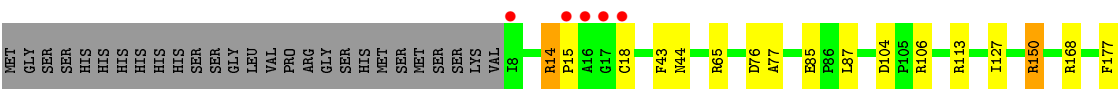
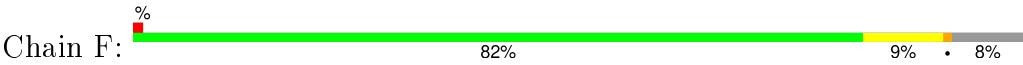


#### • Molecule 1: UHGB\_MP

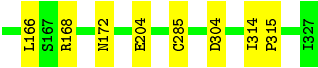
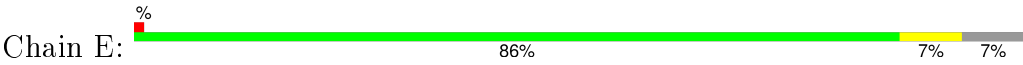




• Molecule 1: UHGB\_MP



• Molecule 2: UHGB\_MP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.74Å 140.89Å 168.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.17 – 1.76 45.43 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.6 (108.17-1.76) 99.6 (45.43-1.76)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.158 , 0.192 0.170 , 0.200	Depositor DCC
$R_{free}$ test set	9952 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 197652 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: GOL, BMA, PO4, EDO, NDG, PGE, K

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	1.19	3/2741 (0.1%)	1.04	15/3736 (0.4%)
1	B	0.96	1/2776 (0.0%)	0.93	5/3785 (0.1%)
1	C	1.00	4/2717 (0.1%)	0.95	5/3703 (0.1%)
1	D	0.91	1/2769 (0.0%)	0.91	5/3772 (0.1%)
1	F	0.92	2/2747 (0.1%)	0.94	8/3744 (0.2%)
2	E	0.96	1/2726 (0.0%)	0.95	3/3716 (0.1%)
All	All	1.00	12/16476 (0.1%)	0.95	41/22456 (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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	TYR	C-N	-35.84	0.51	1.34
1	C	95	GLU	CD-OE1	-7.82	1.17	1.25
1	C	104[A]	ASP	CB-CG	5.60	1.63	1.51
1	C	104[B]	ASP	CB-CG	5.60	1.63	1.51
1	A	271	PRO	N-CD	5.56	1.55	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	TYR	C-N-CA	15.45	160.31	121.70
1	C	323	ARG	NE-CZ-NH1	9.26	124.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	103	TYR	O-C-N	-7.63	110.50	122.70
1	C	323	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	104[B]	ASP	CB-CG-OD2	-6.75	112.22	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104[B]	ASP	Mainchain

## 5.2 Too-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 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	2648	0	2503	18	0
1	B	2686	0	2541	25	0
1	C	2628	0	2476	18	0
1	D	2679	0	2518	26	0
1	F	2657	0	2498	26	0
2	E	2636	0	2482	21	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	12	0	12	6	0
4	B	12	0	10	2	0
4	C	12	0	12	5	0
4	D	12	0	12	6	0
4	E	12	0	12	2	0
4	F	12	0	12	5	0
5	A	15	0	15	1	0
5	B	15	0	14	1	0
5	C	15	0	15	0	0
5	D	15	0	15	0	0
5	E	15	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	15	0	15	0	0
6	A	10	0	14	0	0
6	D	10	0	14	0	0
6	E	10	0	14	2	0
7	A	4	0	6	0	0
7	D	4	0	6	0	0
7	E	4	0	6	0	0
7	F	8	0	12	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	B	6	0	8	0	0
9	C	6	0	8	0	0
10	A	238	0	0	2	0
10	B	226	0	0	1	0
10	C	218	0	0	1	0
10	D	181	0	0	0	0
10	E	188	0	0	0	0
10	F	153	0	0	2	0
All	All	17398	0	15264	133	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 4.

The worst 5 of 133 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:E:44[A]:ASN:ND2	2:E:104[A]:ASP:HA	1.75	1.01
2:E:44[A]:ASN:ND2	2:E:104[A]:ASP:OD1	1.98	0.95
2:E:44[A]:ASN:HD22	2:E:104[A]:ASP:HA	1.31	0.92
1:D:44[A]:ASN:ND2	1:D:104[A]:ASP:HA	1.87	0.88
1:F:44[A]:ASN:HD22	1:F:104[A]:ASP:HA	1.38	0.88

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	329/347 (95%)	314 (95%)	15 (5%)	0	100	100
1	B	333/347 (96%)	317 (95%)	16 (5%)	0	100	100
1	C	324/347 (93%)	309 (95%)	15 (5%)	0	100	100
1	D	332/347 (96%)	315 (95%)	17 (5%)	0	100	100
1	F	330/347 (95%)	316 (96%)	14 (4%)	0	100	100
2	E	327/347 (94%)	308 (94%)	19 (6%)	0	100	100
All	All	1975/2082 (95%)	1879 (95%)	96 (5%)	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	282/298 (95%)	282 (100%)	0	100	100
1	B	288/298 (97%)	287 (100%)	1 (0%)	94	92
1	C	280/298 (94%)	279 (100%)	1 (0%)	93	90
1	D	285/298 (96%)	284 (100%)	1 (0%)	93	90
1	F	282/298 (95%)	281 (100%)	1 (0%)	93	90
2	E	280/298 (94%)	279 (100%)	1 (0%)	93	90
All	All	1697/1788 (95%)	1692 (100%)	5 (0%)	94	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	ARG
1	C	168	ARG
1	D	168	ARG
2	E	168	ARG
1	F	168	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	328	-	4,4,4	0.92	0	6,6,6	0.26	0
4	BMA	A	329	-	12,12,12	1.52	1 (8%)	17,17,17	4.11	8 (47%)
5	NDG	A	330	-	15,15,15	0.97	1 (6%)	17,21,21	1.39	2 (11%)
6	PGE	A	331	-	9,9,9	0.51	0	8,8,8	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	332	-	3,3,3	0.20	0	2,2,2	0.98	0
3	PO4	B	328	-	4,4,4	0.64	0	6,6,6	0.32	0
4	BMA	B	329	1,5	12,12,12	1.14	1 (8%)	17,17,17	3.07	9 (52%)
5	NDG	B	330	4	15,15,15	0.83	1 (6%)	17,21,21	1.43	2 (11%)
9	GOL	B	331	-	5,5,5	0.24	0	5,5,5	0.45	0
3	PO4	C	328	-	4,4,4	1.17	1 (25%)	6,6,6	0.28	0
4	BMA	C	329	-	12,12,12	1.60	1 (8%)	17,17,17	3.84	9 (52%)
5	NDG	C	330	-	15,15,15	1.16	1 (6%)	17,21,21	1.26	2 (11%)
9	GOL	C	331	-	5,5,5	0.82	0	5,5,5	1.56	1 (20%)
3	PO4	D	328	-	4,4,4	0.55	0	6,6,6	0.31	0
4	BMA	D	329	-	12,12,12	1.39	1 (8%)	17,17,17	3.88	9 (52%)
5	NDG	D	330	-	15,15,15	0.71	0	17,21,21	1.51	2 (11%)
6	PGE	D	331	-	9,9,9	0.37	0	8,8,8	0.82	0
7	EDO	D	332	-	3,3,3	0.59	0	2,2,2	0.29	0
3	PO4	E	328	-	4,4,4	0.59	0	6,6,6	0.31	0
4	BMA	E	329	-	12,12,12	1.09	1 (8%)	17,17,17	3.83	9 (52%)
5	NDG	E	330	-	15,15,15	0.76	0	17,21,21	1.30	1 (5%)
6	PGE	E	331	-	9,9,9	0.70	0	8,8,8	1.27	1 (12%)
7	EDO	E	569	-	3,3,3	0.19	0	2,2,2	0.82	0
3	PO4	F	328	-	4,4,4	0.42	0	6,6,6	0.28	0
4	BMA	F	329	-	12,12,12	1.13	1 (8%)	17,17,17	3.37	10 (58%)
5	NDG	F	330	-	15,15,15	0.73	0	17,21,21	1.18	3 (17%)
7	EDO	F	331	-	3,3,3	0.46	0	2,2,2	0.38	0
7	EDO	F	569	-	3,3,3	0.36	0	2,2,2	0.56	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	PO4	A	328	-	-	0/0/0/0	0/0/0/0
4	BMA	A	329	-	-	0/2/22/22	0/1/1/1
5	NDG	A	330	-	-	0/6/26/26	0/1/1/1
6	PGE	A	331	-	-	0/7/7/7	0/0/0/0
7	EDO	A	332	-	-	0/1/1/1	0/0/0/0
3	PO4	B	328	-	-	0/0/0/0	0/0/0/0
4	BMA	B	329	1,5	-	0/2/22/22	0/1/1/1
5	NDG	B	330	4	-	0/6/26/26	0/1/1/1
9	GOL	B	331	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	C	328	-	-	0/0/0/0	0/0/0/0
4	BMA	C	329	-	-	0/2/22/22	0/1/1/1
5	NDG	C	330	-	-	0/6/26/26	0/1/1/1
9	GOL	C	331	-	-	0/4/4/4	0/0/0/0
3	PO4	D	328	-	-	0/0/0/0	0/0/0/0
4	BMA	D	329	-	-	0/2/22/22	0/1/1/1
5	NDG	D	330	-	-	0/6/26/26	0/1/1/1
6	PGE	D	331	-	-	0/7/7/7	0/0/0/0
7	EDO	D	332	-	-	0/1/1/1	0/0/0/0
3	PO4	E	328	-	-	0/0/0/0	0/0/0/0
4	BMA	E	329	-	-	0/2/22/22	0/1/1/1
5	NDG	E	330	-	-	0/6/26/26	0/1/1/1
6	PGE	E	331	-	-	0/7/7/7	0/0/0/0
7	EDO	E	569	-	-	0/1/1/1	0/0/0/0
3	PO4	F	328	-	-	0/0/0/0	0/0/0/0
4	BMA	F	329	-	-	0/2/22/22	0/1/1/1
5	NDG	F	330	-	-	0/6/26/26	0/1/1/1
7	EDO	F	331	-	-	0/1/1/1	0/0/0/0
7	EDO	F	569	-	-	0/1/1/1	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	330	NDG	O7-C7	-3.21	1.15	1.23
5	A	330	NDG	O7-C7	-3.13	1.16	1.23
5	B	330	NDG	O7-C7	-2.29	1.17	1.23
3	C	328	PO4	P-O4	-2.05	1.46	1.53
4	B	329	BMA	O3-C3	2.24	1.48	1.43

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	329	BMA	O1-C1-O5	-7.19	90.58	110.25
4	C	329	BMA	O1-C1-O5	-6.59	92.22	110.25
4	D	329	BMA	O1-C1-O5	-6.15	93.43	110.25
4	A	329	BMA	O1-C1-O5	-5.90	94.11	110.25
4	F	329	BMA	O1-C1-O5	-5.41	95.44	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	329	BMA	6	0
5	A	330	NDG	1	0
4	B	329	BMA	2	0
5	B	330	NDG	1	0
4	C	329	BMA	5	0
4	D	329	BMA	6	0
4	E	329	BMA	2	0
6	E	331	PGE	2	0
4	F	329	BMA	5	0
7	F	331	EDO	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	320/347 (92%)	-0.25	0 100 100	12, 16, 30, 47	0
1	B	320/347 (92%)	-0.24	2 (0%) 90 92	12, 18, 30, 51	0
1	C	319/347 (91%)	-0.27	3 (0%) 85 89	11, 17, 32, 52	0
1	D	320/347 (92%)	-0.15	2 (0%) 90 92	15, 21, 34, 47	0
1	F	320/347 (92%)	-0.03	5 (1%) 74 81	15, 22, 38, 53	0
2	E	321/347 (92%)	-0.16	2 (0%) 90 92	13, 20, 33, 47	0
All	All	1920/2082 (92%)	-0.18	14 (0%) 89 92	11, 19, 34, 53	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	16	ALA	5.4
1	F	17	GLY	4.6
1	D	16	ALA	4.3
2	E	17	GLY	4.2
1	D	17	GLY	3.6

### 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 ⓘ

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
8	K	C	333	1/1	0.96	0.28	27.37	54,54,54,54	0
8	K	B	333	1/1	0.98	0.28	22.76	58,58,58,58	0
9	GOL	C	331	6/6	0.71	0.21	17.18	39,41,46,47	0
8	K	F	333	1/1	0.94	0.26	14.04	62,62,62,62	0
4	BMA	C	329	12/12	0.74	0.37	13.42	22,30,34,37	12
8	K	A	333	1/1	0.98	0.23	12.79	56,56,56,56	0
4	BMA	D	329	12/12	0.64	0.38	10.94	23,28,33,34	12
4	BMA	F	329	12/12	0.65	0.39	10.77	25,31,35,39	12
4	BMA	A	329	12/12	0.67	0.36	10.19	19,26,31,34	12
6	PGE	E	331	10/10	0.86	0.15	9.03	35,42,47,49	0
4	BMA	B	329	12/12	0.65	0.33	8.40	31,50,62,62	0
4	BMA	E	329	12/12	0.72	0.34	7.99	21,27,29,31	12
8	K	E	333	1/1	0.95	0.20	7.65	49,49,49,49	0
6	PGE	D	331	10/10	0.86	0.17	6.57	43,46,61,62	0
6	PGE	A	331	10/10	0.88	0.15	5.52	38,44,47,47	0
7	EDO	A	332	4/4	0.91	0.14	4.71	38,39,42,45	0
5	NDG	C	330	15/15	0.86	0.14	3.28	21,23,25,25	0
9	GOL	B	331	6/6	0.72	0.15	3.22	42,45,47,53	0
5	NDG	B	330	15/15	0.84	0.14	1.68	27,30,32,32	0
7	EDO	F	569	4/4	0.87	0.10	1.25	41,42,42,46	0
5	NDG	A	330	15/15	0.89	0.12	1.22	21,24,27,27	0
5	NDG	F	330	15/15	0.88	0.12	1.21	21,26,27,27	0
5	NDG	E	330	15/15	0.90	0.11	1.03	20,23,25,26	0
5	NDG	D	330	15/15	0.89	0.11	0.18	23,26,27,28	0
3	PO4	B	328	5/5	0.99	0.09	-0.58	14,14,15,18	0
7	EDO	E	569	4/4	0.94	0.07	-0.71	41,41,41,45	0
3	PO4	D	328	5/5	0.99	0.07	-1.12	16,17,18,18	0
3	PO4	E	328	5/5	0.99	0.07	-1.21	14,16,17,17	0
3	PO4	F	328	5/5	0.99	0.06	-1.68	16,16,17,20	0
3	PO4	A	328	5/5	1.00	0.06	-1.78	13,13,14,15	0
3	PO4	C	328	5/5	0.99	0.06	-2.04	13,14,15,16	0
8	K	D	333	1/1	0.95	0.20	-	59,59,59,59	0
7	EDO	F	331	4/4	0.81	0.19	-	40,45,47,53	0
7	EDO	D	332	4/4	0.83	0.19	-	50,54,55,57	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.