



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:15 pm BST

PDB ID : 4UDI  
Title : Crystal structure of b-1,4-mannopyranosyl-chitobiose phosphorylase at 1.85 Angstrom from unknown human gut bacteria (Uhgb\_MP)  
Authors : Ladeveze, S.; Cioci, G.; Potocki-Veronese, G.; Tranier, S.; Mourey, L.  
Deposited on : 2014-12-10  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

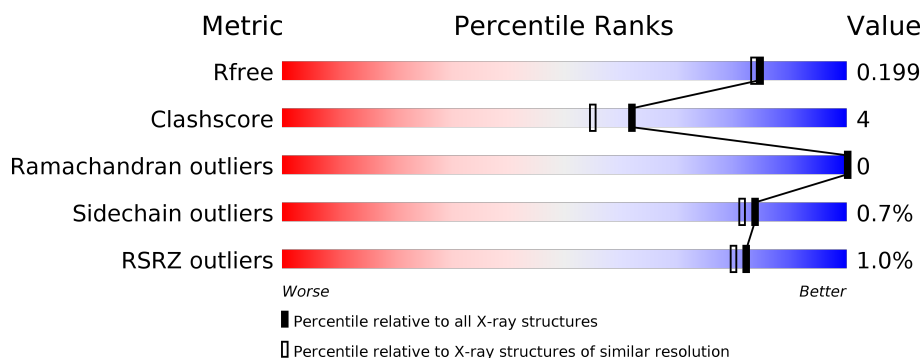
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. 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>%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>7%</div> </div> </div>
1	B	347	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
1	C	347	<div> <div></div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
1	D	347	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>
1	E	347	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
1	F	347	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </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
3	GOL	A	332	-	X	-	-
3	GOL	F	332	-	-	X	-
5	EDO	A	337	-	-	X	-
5	EDO	A	339	-	-	X	-
5	EDO	B	339	-	-	X	-
5	EDO	C	336	-	-	X	-
5	EDO	C	339	-	-	X	-
5	EDO	C	340	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16842 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	321	Total	C	N	O	S	0	5	0
			2601	1683	436	465	17			
1	B	321	Total	C	N	O	S	0	2	0
			2591	1674	435	465	17			
1	C	321	Total	C	N	O	S	0	4	0
			2595	1679	434	465	17			
1	D	320	Total	C	N	O	S	0	1	0
			2558	1652	429	460	17			
1	E	320	Total	C	N	O	S	0	1	0
			2556	1653	428	459	16			
1	F	320	Total	C	N	O	S	0	2	0
			2566	1658	429	462	17			

There are 120 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D9ZDQ9
A	-1	SER	-	expression tag	UNP D9ZDQ9
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

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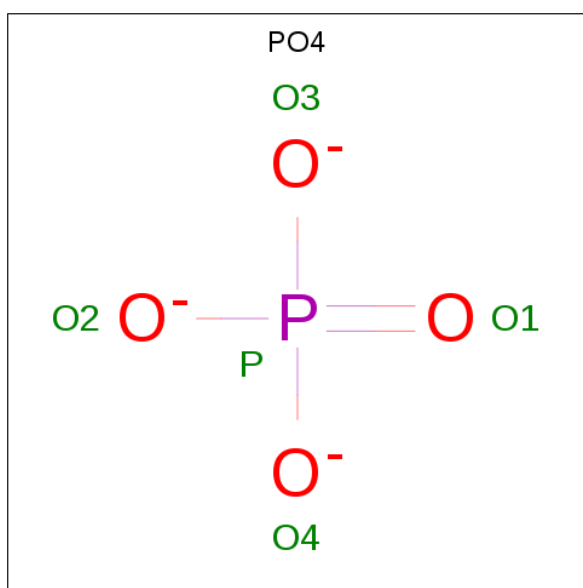
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP D9ZDQ9
D	-19	MET	-	expression tag	UNP D9ZDQ9
D	-18	GLY	-	expression tag	UNP D9ZDQ9
D	-17	SER	-	expression tag	UNP D9ZDQ9
D	-16	SER	-	expression tag	UNP D9ZDQ9
D	-15	HIS	-	expression tag	UNP D9ZDQ9
D	-14	HIS	-	expression tag	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
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
F	-19	MET	-	expression tag	UNP D9ZDQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
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 PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



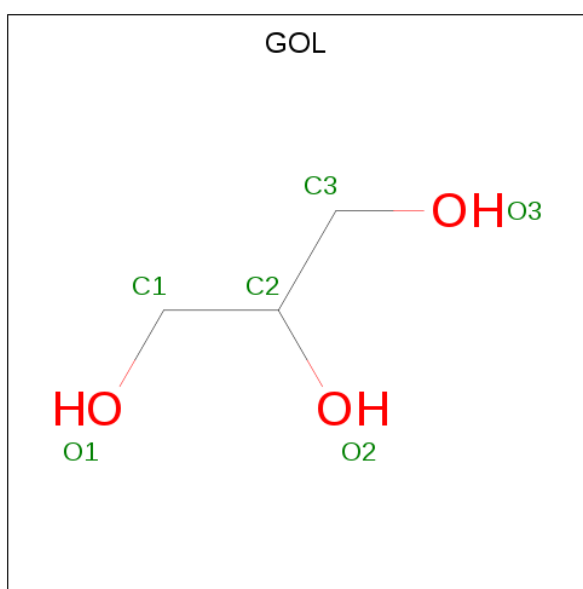
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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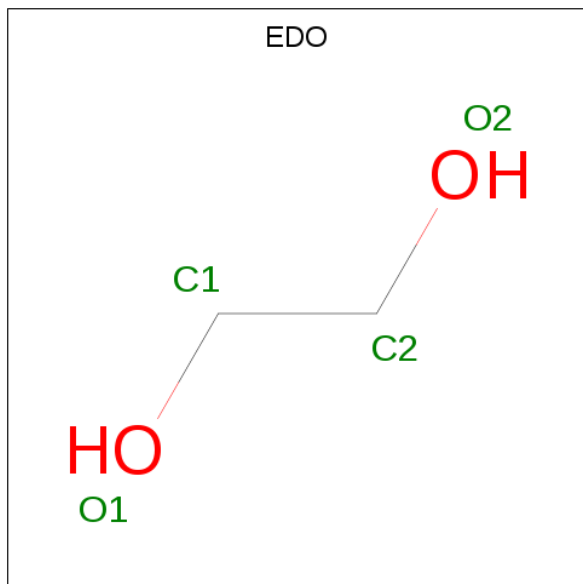
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



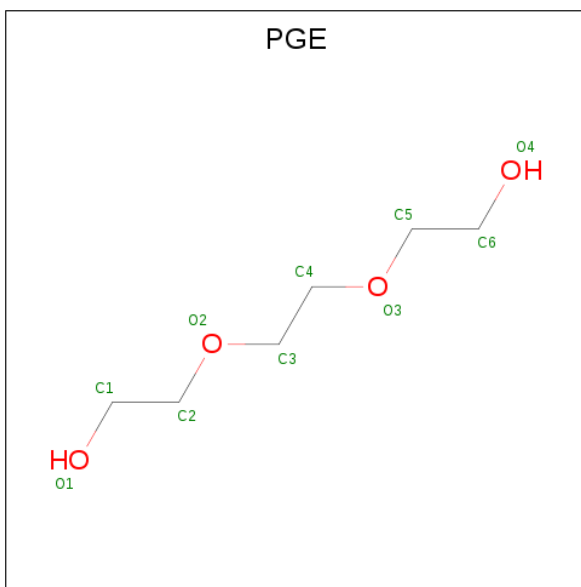
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

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

- 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	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

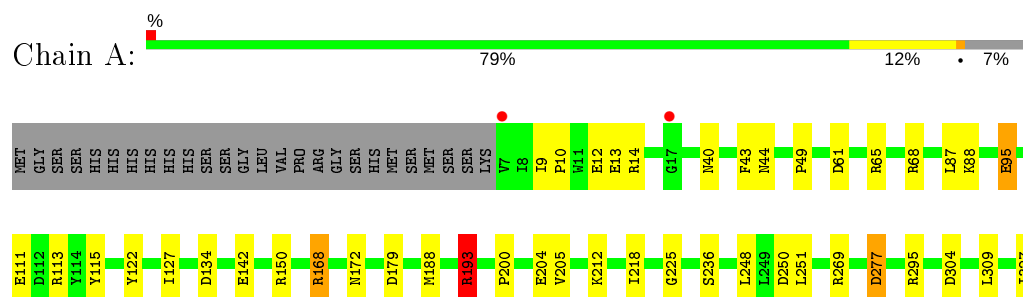
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total	O	0	0
			205	205		
7	B	213	Total	O	0	0
			213	213		
7	C	229	Total	O	0	0
			229	229		
7	D	144	Total	O	0	0
			144	144		
7	E	143	Total	O	0	0
			143	143		
7	F	129	Total	O	0	0
			129	129		

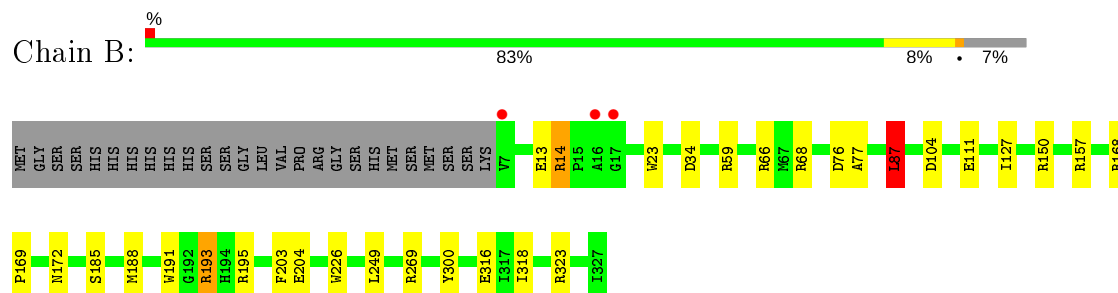
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

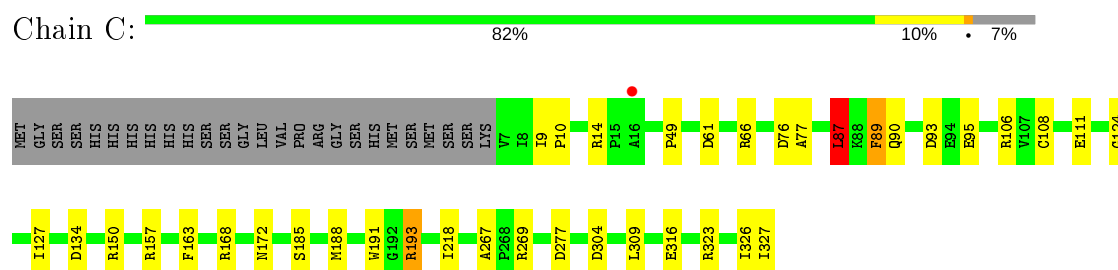
#### • Molecule 1: UHGB\_MP



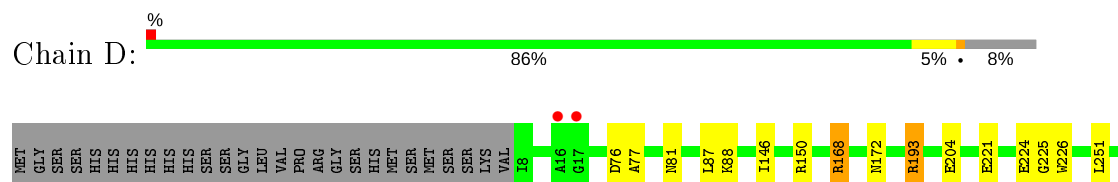
#### • Molecule 1: UHGB\_MP



#### • Molecule 1: UHGB\_MP

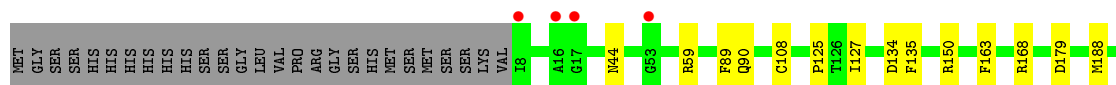
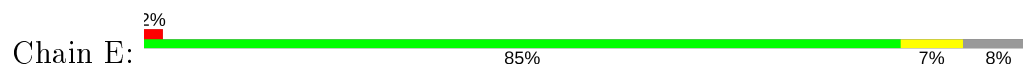


#### • Molecule 1: UHGB\_MP

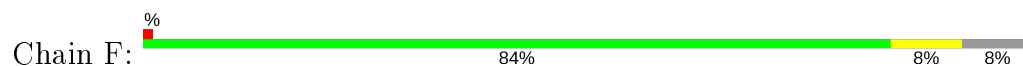




• Molecule 1: UHGB\_MP



• Molecule 1: UHGB\_MP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.12Å 141.21Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.20 – 1.80 48.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (110.20-1.80) 98.1 (48.16-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.155 , 0.190 0.169 , 0.199	Depositor DCC
$R_{free}$ test set	9557 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16842	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 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, K, PGE, EDO

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	1.09	4/2696 (0.1%)	1.11	17/3676 (0.5%)
1	B	1.15	7/2683 (0.3%)	1.08	15/3657 (0.4%)
1	C	1.13	4/2693 (0.1%)	1.10	14/3672 (0.4%)
1	D	0.85	2/2647 (0.1%)	0.94	7/3610 (0.2%)
1	E	0.85	2/2648 (0.1%)	0.99	10/3613 (0.3%)
1	F	0.90	2/2658 (0.1%)	0.98	10/3625 (0.3%)
All	All	1.00	21/16025 (0.1%)	1.04	73/21853 (0.3%)

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	B	0	1
1	C	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	326	ILE	C-N	-16.98	0.94	1.34
1	B	87	LEU	C-N	-10.13	1.10	1.34
1	C	87	LEU	C-N	-9.77	1.11	1.34
1	C	326	ILE	C-N	-8.44	1.14	1.34
1	C	90	GLN	C-N	-7.01	1.18	1.34
1	A	122	TYR	CE2-CZ	6.49	1.47	1.38
1	D	204	GLU	CD-OE1	6.30	1.32	1.25
1	C	89	PHE	C-N	-6.10	1.20	1.34
1	F	18	CYS	C-N	-5.85	1.20	1.34
1	B	13	GLU	CD-OE1	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	TYR	CG-CD2	5.58	1.46	1.39
1	B	300	TYR	CE1-CZ	5.53	1.45	1.38
1	E	204	GLU	CD-OE1	5.50	1.31	1.25
1	A	236	SER	CB-OG	5.42	1.49	1.42
1	A	142	GLU	CD-OE2	-5.42	1.19	1.25
1	D	271	PRO	N-CD	5.11	1.55	1.47
1	E	271	PRO	N-CD	5.11	1.54	1.47
1	B	203	PHE	CB-CG	-5.07	1.42	1.51
1	A	95	GLU	C-N	-5.04	1.22	1.34
1	B	318	ILE	C-N	-5.01	1.22	1.34
1	B	204	GLU	CD-OE1	5.00	1.31	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	GLN	O-C-N	-16.07	96.99	122.70
1	F	193	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	C	90	GLN	O-C-N	-13.76	100.68	122.70
1	F	193	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	A	13	GLU	O-C-N	12.63	142.91	122.70
1	E	90	GLN	CA-C-N	11.45	142.38	117.20
1	E	193	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	13	GLU	CA-C-N	-10.29	94.57	117.20
1	D	193	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	323	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	D	193	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	C	90	GLN	CA-C-N	9.20	137.45	117.20
1	E	193	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	F	17	GLY	C-N-CA	8.55	143.07	121.70
1	F	193	ARG	CG-CD-NE	-8.37	94.22	111.80
1	F	59	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	193	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	193	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	D	193	ARG	CG-CD-NE	-7.80	95.43	111.80
1	E	193	ARG	CG-CD-NE	-7.74	95.55	111.80
1	C	323	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	188	MET	CG-SD-CE	7.48	112.17	100.20
1	D	150	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	260	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	193	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	277	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	C	277	ASP	CB-CG-OD2	-7.10	111.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	87	LEU	O-C-N	-6.75	111.90	122.70
1	B	14[A]	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	B	14[B]	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	113	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	F	59	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	193	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	106	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	188	MET	CG-SD-CE	6.41	110.46	100.20
1	A	188	MET	CG-SD-CE	6.37	110.39	100.20
1	A	327	ILE	CB-CA-C	-6.17	99.26	111.60
1	F	17	GLY	O-C-N	-6.11	112.93	122.70
1	B	59	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	68	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	134	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	248	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	B	87	LEU	O-C-N	-5.81	113.40	122.70
1	C	193	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	89	PHE	O-C-N	5.74	131.88	122.70
1	A	134	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	68	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	14[A]	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	14[B]	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	179	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	B	34	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	250	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	12	GLU	O-C-N	-5.60	113.74	122.70
1	D	270	GLU	C-N-CD	5.60	140.15	128.40
1	B	104	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	E	179	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	309	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	106	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	168	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	E	270	GLU	C-N-CD	5.38	139.71	128.40
1	F	193	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	323	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	13	GLU	C-N-CA	-5.33	108.38	121.70
1	F	157	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	168	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	F	134	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	61	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	195	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	90	GLN	C-N-CA	5.07	134.38	121.70
1	E	277	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	C	309	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	LEU	Mainchain
1	C	87	LEU	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	2601	0	2465	33	0
1	B	2591	0	2460	23	0
1	C	2595	0	2461	27	0
1	D	2558	0	2400	11	0
1	E	2556	0	2403	12	0
1	F	2566	0	2407	16	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	24	0	32	4	0
3	B	36	0	48	6	0
3	C	36	0	48	6	0
3	D	24	0	32	3	0
3	E	12	0	16	2	0
3	F	30	0	40	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	28	0	41	12	0
5	B	8	0	12	6	0
5	C	24	0	36	20	0
5	D	4	0	6	0	0
5	E	12	0	18	1	0
5	F	8	0	12	2	0
6	A	10	0	14	3	0
6	B	10	0	14	0	0
6	C	10	0	14	1	0
7	A	205	0	0	8	1
7	B	213	0	0	1	0
7	C	229	0	0	6	1
7	D	144	0	0	1	0
7	E	143	0	0	1	0
7	F	129	0	0	1	0
All	All	16842	0	14979	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (135) 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:A:277:ASP:OD1	5:C:336:EDO:H21	1.70	0.90
1:C:269:ARG:HD3	3:C:335:GOL:H12	1.54	0.87
1:A:14[A]:ARG:HH11	1:A:14[A]:ARG:HG3	1.40	0.87
1:D:172:ASN:HB2	3:D:332:GOL:O1	1.74	0.87
1:C:163:PHE:HZ	5:C:340:EDO:H11	1.45	0.82
1:E:125:PRO:HD3	3:E:332:GOL:H2	1.61	0.82
1:A:172:ASN:O	3:A:332:GOL:H31	1.80	0.82
5:A:346:EDO:H21	7:A:465:HOH:O	1.81	0.79
1:B:111:GLU:CG	5:B:339:EDO:H11	2.16	0.76
1:C:163:PHE:CZ	5:C:340:EDO:H11	2.21	0.75
6:A:341:PGE:H12	7:A:574:HOH:O	1.85	0.75
1:A:14[A]:ARG:NH1	1:A:14[A]:ARG:HG3	2.00	0.75
1:C:267:ALA:HB3	5:C:336:EDO:H11	1.69	0.75
1:E:127[A]:ILE:HD11	1:E:150:ARG:HA	1.67	0.74
1:A:111:GLU:HG2	5:A:339:EDO:H11	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:NH1	5:B:346:EDO:H21	2.03	0.73
1:B:127:ILE:HD11	1:B:150:ARG:HA	1.72	0.71
1:D:172:ASN:CB	3:D:332:GOL:O1	2.39	0.71
1:B:111:GLU:HG3	5:B:339:EDO:H11	1.73	0.70
1:A:269:ARG:HD3	3:A:335:GOL:H12	1.75	0.68
1:A:111:GLU:CG	5:A:339:EDO:H11	2.23	0.68
1:B:14[A]:ARG:NH2	1:B:316:GLU:OE1	2.28	0.67
1:B:269:ARG:HD3	3:B:335:GOL:H12	1.76	0.66
1:D:81:ASN:HB3	7:D:553:HOH:O	1.94	0.66
1:F:41:SER:OG	5:F:337:EDO:H22	1.95	0.66
1:F:172:ASN:HB2	3:F:332:GOL:O1	1.97	0.65
1:C:49:PRO:HD2	6:C:341:PGE:H52	1.79	0.65
1:E:127[A]:ILE:CD1	1:E:150:ARG:HA	2.29	0.63
5:A:346:EDO:C2	7:A:465:HOH:O	2.40	0.63
1:F:304:ASP:O	5:F:337:EDO:O2	2.15	0.60
1:A:193:ARG:NH2	5:E:573:EDO:O1	2.35	0.60
3:A:330:GOL:H32	7:A:434:HOH:O	2.00	0.59
1:B:111:GLU:HG2	5:B:339:EDO:H11	1.84	0.59
1:C:14[A]:ARG:NH2	1:C:316:GLU:OE2	2.35	0.59
1:C:267:ALA:CB	5:C:336:EDO:H11	2.33	0.58
1:B:172:ASN:HA	3:B:332:GOL:H31	1.86	0.58
1:C:127[A]:ILE:HD11	1:C:150:ARG:HA	1.86	0.58
1:B:14[B]:ARG:HH11	1:B:14[B]:ARG:HG3	1.68	0.58
1:A:127[A]:ILE:HD11	1:A:150:ARG:HA	1.87	0.57
1:C:157:ARG:HA	5:C:339:EDO:H12	1.87	0.57
5:C:347:EDO:H11	7:C:552:HOH:O	2.05	0.56
1:C:111:GLU:HG3	5:C:339:EDO:H11	1.86	0.56
1:B:172:ASN:HB2	3:B:332:GOL:O3	2.06	0.56
1:B:14[B]:ARG:NH1	1:B:14[B]:ARG:HG3	2.20	0.56
1:C:269:ARG:CD	3:C:335:GOL:H12	2.34	0.55
6:A:341:PGE:C1	7:A:574:HOH:O	2.49	0.55
1:B:172:ASN:CA	3:B:332:GOL:H31	2.37	0.55
1:A:115:TYR:OH	5:A:597:EDO:H11	2.07	0.54
1:A:95:GLU:OE2	7:E:494:HOH:O	2.17	0.54
1:B:87:LEU:O	3:B:334:GOL:H11	2.08	0.54
1:C:124:GLY:HA2	3:C:332:GOL:H2	1.90	0.54
1:A:40:ASN:OD1	5:C:336:EDO:H22	2.07	0.53
1:A:304:ASP:O	5:A:337:EDO:O1	2.26	0.53
1:A:269:ARG:HD3	3:A:335:GOL:C1	2.38	0.53
3:C:330:GOL:H32	7:C:434:HOH:O	2.07	0.53
1:A:225:GLY:HA2	1:A:251:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:HD22	1:A:105:PRO:HD2	1.73	0.53
5:C:336:EDO:O2	7:C:533:HOH:O	2.19	0.52
1:D:172:ASN:HB2	3:D:332:GOL:HO1	1.69	0.52
1:C:66:ARG:HH12	5:C:343:EDO:C1	2.23	0.51
1:C:111:GLU:CG	5:C:339:EDO:H11	2.40	0.51
1:F:44:ASN:HD22	1:F:105:PRO:HD2	1.74	0.51
1:B:157:ARG:HB2	5:B:339:EDO:H21	1.93	0.50
1:F:172:ASN:CB	3:F:332:GOL:O1	2.60	0.50
1:E:108:CYS:HB3	1:E:218:ILE:HG13	1.94	0.50
1:E:44:ASN:HB2	1:E:59:ARG:HB3	1.94	0.49
1:C:157:ARG:CB	5:C:339:EDO:H12	2.43	0.49
1:F:127[A]:ILE:CD1	1:F:150:ARG:HA	2.42	0.49
1:F:101:TYR:HH	3:F:332:GOL:HO3	1.49	0.49
1:E:125:PRO:CD	3:E:332:GOL:H2	2.38	0.49
1:A:127[A]:ILE:CD1	1:A:150:ARG:HA	2.42	0.49
1:F:127[A]:ILE:HD11	1:F:150:ARG:HA	1.95	0.49
1:D:225:GLY:HA2	1:D:251:LEU:HD13	1.95	0.48
1:E:127[A]:ILE:HD11	1:E:150:ARG:CA	2.42	0.48
1:B:226:TRP:HB2	1:B:249:LEU:HB2	1.97	0.47
1:C:66:ARG:HH22	5:C:343:EDO:C2	2.27	0.47
1:F:163:PHE:CD1	1:F:188:MET:HE1	2.49	0.46
1:A:277:ASP:OD1	5:C:336:EDO:C2	2.55	0.46
1:A:108:CYS:HB3	1:A:218:ILE:HG13	1.98	0.46
1:C:172:ASN:HB2	3:C:332:GOL:O3	2.16	0.45
1:D:224:GLU:OE1	1:D:322:LYS:NZ	2.47	0.45
1:C:108:CYS:HB3	1:C:218:ILE:HG13	1.98	0.45
1:B:157:ARG:HA	5:B:339:EDO:H12	1.99	0.45
5:C:340:EDO:H22	7:C:403:HOH:O	2.17	0.45
1:C:87:LEU:HD11	1:C:89:PHE:CZ	2.52	0.45
1:A:49:PRO:HD2	6:A:341:PGE:H4	1.98	0.45
1:A:14[A]:ARG:HH11	1:A:14[A]:ARG:CG	2.13	0.45
1:D:76:ASP:O	1:D:77:ALA:HB3	2.17	0.45
1:A:87:LEU:HD23	1:A:88:LYS:N	2.32	0.45
1:A:43:PHE:CZ	5:A:337:EDO:H21	2.52	0.45
3:B:335:GOL:H2	7:B:396:HOH:O	2.17	0.44
1:C:93:ASP:OD1	1:C:95:GLU:HB3	2.17	0.44
1:A:43:PHE:CE1	5:A:337:EDO:H21	2.52	0.44
1:A:204[A]:GLU:HG2	1:A:205:VAL:HG23	1.99	0.44
1:F:299:TYR:CE2	1:F:309:LEU:HD13	2.53	0.44
1:B:269:ARG:HG2	5:C:347:EDO:H22	2.00	0.44
1:C:76:ASP:O	1:C:77:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:SER:HA	1:F:175:THR:HG21	2.00	0.44
1:A:9:ILE:HB	1:A:10:PRO:HD2	1.99	0.44
1:A:61:ASP:OD2	5:A:337:EDO:H22	2.17	0.44
1:E:163:PHE:CD1	1:E:188:MET:HE1	2.53	0.43
1:A:111:GLU:HG3	5:A:339:EDO:H11	1.99	0.43
1:C:185:SER:HB2	1:C:191:TRP:CD2	2.54	0.43
5:C:347:EDO:C1	7:C:552:HOH:O	2.65	0.43
1:C:127[A]:ILE:CD1	1:C:150:ARG:HA	2.48	0.43
1:A:87:LEU:C	1:A:87:LEU:HD23	2.38	0.43
1:B:14[A]:ARG:HB2	1:B:23:TRP:CH2	2.53	0.43
1:F:200:PRO:HG3	1:F:212:LYS:HA	1.99	0.43
1:F:217:PRO:HD2	1:F:229:ILE:HB	1.99	0.43
1:A:200:PRO:HG3	1:A:212:LYS:HA	2.01	0.42
1:A:295:ARG:NH1	7:A:516:HOH:O	2.44	0.42
1:B:127:ILE:CD1	1:B:150:ARG:HA	2.43	0.42
1:B:76:ASP:O	1:B:77:ALA:HB3	2.20	0.42
1:D:221:GLU:HB2	1:D:226:TRP:CZ3	2.55	0.42
1:A:65:ARG:NH2	5:A:337:EDO:C1	2.83	0.42
1:A:44:ASN:ND2	7:A:419:HOH:O	2.32	0.42
1:B:169:PRO:HG3	1:D:146:ILE:CG2	2.50	0.42
1:E:134:ASP:O	1:E:135:PHE:HB2	2.19	0.42
3:C:331:GOL:O1	5:C:340:EDO:C1	2.68	0.41
1:D:292:GLU:HA	1:D:292:GLU:OE1	2.20	0.41
3:F:332:GOL:H31	7:F:498:HOH:O	2.19	0.41
1:F:146:ILE:HG21	1:F:146:ILE:HD13	1.80	0.41
1:C:14[B]:ARG:NH2	1:C:316:GLU:OE1	2.49	0.41
1:C:327:ILE:CG2	7:C:547:HOH:O	2.69	0.41
1:F:278:VAL:O	1:F:303:ALA:HA	2.19	0.41
1:B:14[B]:ARG:CG	1:B:14[B]:ARG:HH11	2.33	0.41
1:E:225:GLY:HA2	1:E:251:LEU:HG	2.03	0.41
5:A:339:EDO:C1	7:A:405:HOH:O	2.69	0.41
1:F:275:MET:HB2	1:F:275:MET:HE2	1.86	0.41
1:C:66:ARG:HH22	5:C:343:EDO:H22	1.85	0.41
1:D:87:LEU:HD23	1:D:88:LYS:N	2.36	0.41
1:E:222:THR:HG21	1:E:318:ILE:HD11	2.03	0.40
1:C:9:ILE:HB	1:C:10:PRO:HD2	2.04	0.40
1:E:163:PHE:CD1	1:E:188:MET:CE	3.05	0.40
1:B:185:SER:HB2	1:B:191:TRP:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:505:HOH:O	7:C:390:HOH:O[1_455]	1.79	0.41

## 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	324/347 (93%)	305 (94%)	19 (6%)	0	100	100
1	B	321/347 (92%)	298 (93%)	23 (7%)	0	100	100
1	C	323/347 (93%)	302 (94%)	21 (6%)	0	100	100
1	D	319/347 (92%)	302 (95%)	17 (5%)	0	100	100
1	E	319/347 (92%)	302 (95%)	17 (5%)	0	100	100
1	F	320/347 (92%)	304 (95%)	16 (5%)	0	100	100
All	All	1926/2082 (92%)	1813 (94%)	113 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	276/298 (93%)	274 (99%)	2 (1%)	84	81
1	B	277/298 (93%)	275 (99%)	2 (1%)	84	81
1	C	277/298 (93%)	275 (99%)	2 (1%)	84	81
1	D	270/298 (91%)	268 (99%)	2 (1%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	269/298 (90%)	268 (100%)	1 (0%)	91	89
1	F	271/298 (91%)	269 (99%)	2 (1%)	84	81
All	All	1640/1788 (92%)	1629 (99%)	11 (1%)	84	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ARG
1	A	193	ARG
1	B	168	ARG
1	B	193	ARG
1	C	168	ARG
1	C	193	ARG
1	D	168	ARG
1	D	193	ARG
1	E	168	ARG
1	F	168	ARG
1	F	193	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 63 ligands modelled in this entry, 6 are monoatomic - leaving 57 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$
6	PGE	B	341	-	9,9,9	0.73	0	8,8,8	0.69	0
3	GOL	E	329	-	5,5,5	0.25	0	5,5,5	0.39	0
5	EDO	A	346	-	3,3,3	0.52	0	2,2,2	0.74	0
3	GOL	C	335	-	5,5,5	1.00	0	5,5,5	0.83	0
2	PO4	F	328	-	4,4,4	0.75	0	6,6,6	1.07	0
3	GOL	C	331	-	5,5,5	0.76	0	5,5,5	0.87	0
5	EDO	E	570	-	3,3,3	0.51	0	2,2,2	0.60	0
3	GOL	D	331	-	5,5,5	0.43	0	5,5,5	1.07	0
3	GOL	C	334	-	5,5,5	0.35	0	5,5,5	0.86	0
5	EDO	A	569	-	3,3,3	0.69	0	2,2,2	0.28	0
3	GOL	F	334	-	5,5,5	0.39	0	5,5,5	0.84	0
5	EDO	A	339	-	3,3,3	0.22	0	2,2,2	0.50	0
3	GOL	D	329	-	5,5,5	0.30	0	5,5,5	0.60	0
6	PGE	A	341	-	9,9,9	0.75	0	8,8,8	0.59	0
3	GOL	C	332	-	5,5,5	0.52	0	5,5,5	0.79	0
5	EDO	A	597	-	3,3,3	0.55	0	2,2,2	0.89	0
3	GOL	A	332	-	5,5,5	0.63	0	5,5,5	1.72	2 (40%)
5	EDO	E	569	-	3,3,3	0.38	0	2,2,2	1.45	0
2	PO4	C	328	-	4,4,4	1.31	0	6,6,6	1.47	1 (16%)
5	EDO	B	346	-	3,3,3	0.68	0	2,2,2	0.28	0
5	EDO	C	340	-	3,3,3	0.55	0	2,2,2	0.69	0
3	GOL	B	331	-	5,5,5	0.40	0	5,5,5	1.43	0
3	GOL	A	330	-	5,5,5	0.60	0	5,5,5	0.66	0
3	GOL	B	334	-	5,5,5	0.32	0	5,5,5	1.77	1 (20%)
5	EDO	A	348	-	3,3,3	0.67	0	2,2,2	0.27	0
3	GOL	A	335	-	5,5,5	1.01	0	5,5,5	1.59	1 (20%)
5	EDO	C	347	-	3,3,3	0.66	0	2,2,2	0.84	0
3	GOL	E	332	-	5,5,5	0.84	0	5,5,5	1.59	1 (20%)
3	GOL	F	332	-	5,5,5	0.37	0	5,5,5	0.73	0
5	EDO	A	345	-	3,3,3	0.54	0	2,2,2	1.42	0
5	EDO	C	339	-	3,3,3	0.14	0	2,2,2	1.02	0
2	PO4	D	328	-	4,4,4	0.59	0	6,6,6	0.63	0
3	GOL	B	332	-	5,5,5	0.60	0	5,5,5	1.35	1 (20%)
5	EDO	C	344	-	3,3,3	0.41	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	339	-	3,3,3	0.59	0	2,2,2	0.68	0
5	EDO	C	336	-	3,3,3	0.39	0	2,2,2	1.26	0
3	GOL	B	330	-	5,5,5	0.84	0	5,5,5	0.55	0
5	EDO	D	339	-	3,3,3	0.29	0	2,2,2	0.52	0
3	GOL	C	329	-	5,5,5	0.31	0	5,5,5	0.76	0
3	GOL	A	329	-	5,5,5	0.40	0	5,5,5	0.45	0
3	GOL	D	330	-	5,5,5	0.30	0	5,5,5	0.90	0
3	GOL	F	330	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	C	330	-	5,5,5	0.46	0	5,5,5	0.69	0
3	GOL	F	329	-	5,5,5	0.28	0	5,5,5	0.60	0
5	EDO	E	573	-	3,3,3	0.45	0	2,2,2	0.93	0
2	PO4	B	328	-	4,4,4	0.92	0	6,6,6	0.86	0
6	PGE	C	341	-	9,9,9	0.99	0	8,8,8	1.58	2 (25%)
3	GOL	F	335	-	5,5,5	0.59	0	5,5,5	0.49	0
3	GOL	B	329	-	5,5,5	0.29	0	5,5,5	0.59	0
2	PO4	E	328	-	4,4,4	1.55	1 (25%)	6,6,6	1.40	1 (16%)
3	GOL	D	332	-	5,5,5	0.62	0	5,5,5	1.88	2 (40%)
5	EDO	F	337	-	3,3,3	0.15	0	2,2,2	0.52	0
5	EDO	F	570	-	3,3,3	0.41	0	2,2,2	0.80	0
3	GOL	B	335	-	5,5,5	0.63	0	5,5,5	1.13	0
2	PO4	A	328	-	4,4,4	1.31	0	6,6,6	1.12	0
5	EDO	C	343	-	3,3,3	0.31	0	2,2,2	1.22	0
5	EDO	A	337	-	3,3,3	1.02	0	2,2,2	0.55	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
6	PGE	B	341	-	-	3/7/7/7	-
3	GOL	E	329	-	-	0/4/4/4	-
5	EDO	A	346	-	-	1/1/1/1	-
3	GOL	C	335	-	-	4/4/4/4	-
3	GOL	C	331	-	-	2/4/4/4	-
5	EDO	E	570	-	-	0/1/1/1	-
3	GOL	D	331	-	-	2/4/4/4	-
3	GOL	C	334	-	-	4/4/4/4	-
5	EDO	A	569	-	-	1/1/1/1	-
3	GOL	F	334	-	-	2/4/4/4	-
5	EDO	A	339	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	330	-	-	2/4/4/4	-
6	PGE	A	341	-	-	2/7/7/7	-
3	GOL	C	332	-	-	4/4/4/4	-
5	EDO	A	597	-	-	1/1/1/1	-
3	GOL	A	332	-	-	4/4/4/4	-
5	EDO	E	569	-	-	1/1/1/1	-
5	EDO	B	346	-	-	0/1/1/1	-
5	EDO	C	340	-	-	0/1/1/1	-
3	GOL	B	331	-	-	0/4/4/4	-
3	GOL	A	330	-	-	2/4/4/4	-
3	GOL	B	334	-	-	2/4/4/4	-
5	EDO	A	348	-	-	1/1/1/1	-
3	GOL	A	335	-	-	4/4/4/4	-
5	EDO	C	347	-	-	1/1/1/1	-
3	GOL	E	332	-	-	4/4/4/4	-
3	GOL	F	332	-	-	4/4/4/4	-
5	EDO	A	345	-	-	0/1/1/1	-
5	EDO	C	339	-	-	0/1/1/1	-
3	GOL	B	332	-	-	2/4/4/4	-
5	EDO	C	344	-	-	1/1/1/1	-
5	EDO	B	339	-	-	0/1/1/1	-
5	EDO	C	336	-	-	0/1/1/1	-
3	GOL	F	335	-	-	0/4/4/4	-
5	EDO	D	339	-	-	1/1/1/1	-
3	GOL	C	329	-	-	0/4/4/4	-
3	GOL	A	329	-	-	0/4/4/4	-
3	GOL	D	330	-	-	0/4/4/4	-
3	GOL	F	330	-	-	2/4/4/4	-
3	GOL	C	330	-	-	1/4/4/4	-
3	GOL	F	329	-	-	0/4/4/4	-
5	EDO	E	573	-	-	1/1/1/1	-
5	EDO	F	570	-	-	1/1/1/1	-
6	PGE	C	341	-	-	2/7/7/7	-
3	GOL	B	329	-	-	2/4/4/4	-
3	GOL	D	329	-	-	0/4/4/4	-
3	GOL	D	332	-	-	3/4/4/4	-
5	EDO	F	337	-	-	0/1/1/1	-
3	GOL	B	335	-	-	4/4/4/4	-
5	EDO	C	343	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	337	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	328	PO4	P-O1	2.84	1.57	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	334	GOL	O3-C3-C2	-3.39	93.93	110.20
6	C	341	PGE	O3-C5-C6	3.18	124.02	110.07
3	A	332	GOL	C3-C2-C1	-3.08	99.74	111.70
3	D	332	GOL	O1-C1-C2	-3.02	95.70	110.20
3	E	332	GOL	O2-C2-C3	3.00	122.32	109.12
3	A	335	GOL	O1-C1-C2	2.84	123.83	110.20
2	C	328	PO4	O4-P-O2	2.84	117.08	107.97
3	D	332	GOL	O3-C3-C2	-2.61	97.70	110.20
6	C	341	PGE	O4-C6-C5	2.44	125.96	111.81
3	B	332	GOL	C3-C2-C1	-2.36	102.51	111.70
2	E	328	PO4	O4-P-O1	-2.16	102.98	110.89
3	A	332	GOL	O2-C2-C1	2.09	118.31	109.12

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	331	GOL	C1-C2-C3-O3
3	D	331	GOL	O2-C2-C3-O3
3	C	334	GOL	O1-C1-C2-O2
3	C	334	GOL	O1-C1-C2-C3
3	F	334	GOL	C1-C2-C3-O3
3	C	335	GOL	O1-C1-C2-C3
3	C	335	GOL	C1-C2-C3-O3
3	C	332	GOL	C1-C2-C3-O3
3	A	332	GOL	O1-C1-C2-C3
3	A	330	GOL	C1-C2-C3-O3
3	B	334	GOL	O1-C1-C2-C3
3	A	335	GOL	O1-C1-C2-C3
3	A	335	GOL	C1-C2-C3-O3
3	E	332	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	F	332	GOL	O1-C1-C2-C3
3	F	332	GOL	C1-C2-C3-O3
3	F	330	GOL	C1-C2-C3-O3
3	D	332	GOL	C1-C2-C3-O3
3	D	332	GOL	O2-C2-C3-O3
3	B	335	GOL	C1-C2-C3-O3
6	C	341	PGE	O2-C3-C4-O3
3	A	335	GOL	O1-C1-C2-O2
3	A	335	GOL	O2-C2-C3-O3
6	B	341	PGE	O1-C1-C2-O2
3	B	330	GOL	O1-C1-C2-C3
3	C	331	GOL	C1-C2-C3-O3
3	C	334	GOL	C1-C2-C3-O3
3	C	332	GOL	O1-C1-C2-C3
3	A	332	GOL	C1-C2-C3-O3
3	E	332	GOL	O1-C1-C2-C3
3	B	332	GOL	O1-C1-C2-C3
3	B	329	GOL	C1-C2-C3-O3
3	B	335	GOL	O1-C1-C2-C3
6	A	341	PGE	O1-C1-C2-O2
3	C	334	GOL	O2-C2-C3-O3
3	F	334	GOL	O2-C2-C3-O3
3	C	335	GOL	O2-C2-C3-O3
3	C	332	GOL	O1-C1-C2-O2
3	A	332	GOL	O1-C1-C2-O2
3	B	334	GOL	O1-C1-C2-O2
3	E	332	GOL	O1-C1-C2-O2
3	F	332	GOL	O1-C1-C2-O2
3	F	332	GOL	O2-C2-C3-O3
3	F	330	GOL	O2-C2-C3-O3
3	B	335	GOL	O2-C2-C3-O3
5	D	339	EDO	O1-C1-C2-O2
6	B	341	PGE	O2-C3-C4-O3
6	B	341	PGE	O3-C5-C6-O4
3	C	331	GOL	O2-C2-C3-O3
3	C	335	GOL	O1-C1-C2-O2
3	C	332	GOL	O2-C2-C3-O3
5	C	347	EDO	O1-C1-C2-O2
5	E	573	EDO	O1-C1-C2-O2
3	B	332	GOL	O1-C1-C2-O2
3	B	335	GOL	O1-C1-C2-O2
5	A	346	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	348	EDO	O1-C1-C2-O2
5	F	570	EDO	O1-C1-C2-O2
3	E	332	GOL	O2-C2-C3-O3
5	C	344	EDO	O1-C1-C2-O2
3	A	330	GOL	O2-C2-C3-O3
3	D	332	GOL	O1-C1-C2-O2
6	A	341	PGE	O2-C3-C4-O3
6	C	341	PGE	C3-C4-O3-C5
5	E	569	EDO	O1-C1-C2-O2
5	A	569	EDO	O1-C1-C2-O2
5	A	597	EDO	O1-C1-C2-O2
3	B	330	GOL	O1-C1-C2-O2
3	A	332	GOL	O2-C2-C3-O3
3	B	329	GOL	O2-C2-C3-O3
3	C	330	GOL	C1-C2-C3-O3

There are no ring outliers.

28 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	346	EDO	2	0
3	C	335	GOL	2	0
3	C	331	GOL	1	0
5	A	339	EDO	4	0
6	A	341	PGE	3	0
3	C	332	GOL	2	0
5	A	597	EDO	1	0
3	A	332	GOL	1	0
5	B	346	EDO	1	0
5	C	340	EDO	4	0
3	A	330	GOL	1	0
3	B	334	GOL	1	0
3	A	335	GOL	2	0
5	C	347	EDO	3	0
3	E	332	GOL	2	0
3	F	332	GOL	4	0
5	C	339	EDO	4	0
3	B	332	GOL	3	0
5	B	339	EDO	5	0
5	C	336	EDO	6	0
3	C	330	GOL	1	0
5	E	573	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	341	PGE	1	0
3	D	332	GOL	3	0
5	F	337	EDO	2	0
3	B	335	GOL	2	0
5	C	343	EDO	3	0
5	A	337	EDO	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
1	B	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	89:PHE	C	90:GLN	N	1.20
1	C	90:GLN	C	91:CYS	N	1.17
1	C	326:ILE	C	327:ILE	N	1.14
1	C	87:LEU	C	88:LYS	N	1.11
1	B	87:LEU	C	88:LYS	N	1.10
1	F	326:ILE	C	327:ILE	N	0.95



## 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	321/347 (92%)	-0.49	2 (0%) 89 87	18, 26, 43, 66	0
1	B	321/347 (92%)	-0.42	3 (0%) 84 82	17, 25, 42, 57	0
1	C	321/347 (92%)	-0.51	1 (0%) 94 92	18, 25, 43, 63	0
1	D	320/347 (92%)	-0.29	4 (1%) 77 74	24, 39, 59, 82	0
1	E	320/347 (92%)	-0.25	6 (1%) 66 63	26, 40, 63, 81	0
1	F	320/347 (92%)	-0.31	3 (0%) 84 82	25, 40, 60, 82	0
All	All	1923/2082 (92%)	-0.38	19 (0%) 82 80	17, 32, 58, 82	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	ALA	3.4
1	D	16	ALA	3.3
1	E	327	ILE	2.9
1	D	17	GLY	2.7
1	F	17	GLY	2.7
1	A	7	VAL	2.7
1	F	16	ALA	2.7
1	E	17	GLY	2.7
1	A	17	GLY	2.6
1	E	8	ILE	2.5
1	B	16	ALA	2.4
1	B	17	GLY	2.3
1	D	327	ILE	2.3
1	B	7	VAL	2.3
1	E	223	PRO	2.2
1	C	16	ALA	2.2
1	D	292	GLU	2.1
1	E	53	GLY	2.1
1	F	292	GLU	2.0

## 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 ⓘ

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	PGE	A	341	10/10	0.69	0.21	44,58,69,73	0
5	EDO	A	345	4/4	0.73	0.14	56,58,59,64	0
6	PGE	B	341	10/10	0.75	0.19	43,62,67,69	0
5	EDO	A	348	4/4	0.79	0.22	53,57,58,62	0
5	EDO	A	597	4/4	0.80	0.13	56,57,59,67	0
5	EDO	E	569	4/4	0.81	0.14	55,60,61,65	0
3	GOL	D	331	6/6	0.84	0.14	59,60,61,62	0
3	GOL	C	335	6/6	0.85	0.20	36,46,52,53	0
3	GOL	E	332	6/6	0.85	0.17	47,49,51,57	0
3	GOL	C	331	6/6	0.85	0.19	53,56,59,61	0
3	GOL	F	335	6/6	0.85	0.17	58,66,67,71	0
6	PGE	C	341	10/10	0.85	0.21	36,58,62,62	0
3	GOL	A	332	6/6	0.85	0.15	46,52,56,58	0
3	GOL	F	334	6/6	0.86	0.15	56,58,62,62	0
3	GOL	F	330	6/6	0.86	0.22	55,64,66,67	0
3	GOL	D	329	6/6	0.88	0.13	41,45,46,49	0
5	EDO	E	570	4/4	0.89	0.12	57,58,60,63	0
3	GOL	D	330	6/6	0.89	0.19	55,58,59,60	0
5	EDO	C	343	4/4	0.89	0.36	45,48,53,54	0
3	GOL	F	329	6/6	0.90	0.10	43,45,47,48	0
5	EDO	E	573	4/4	0.90	0.12	54,59,61,65	0
4	K	F	333	1/1	0.90	0.23	63,63,63,63	0
3	GOL	B	334	6/6	0.90	0.14	43,48,51,52	0
3	GOL	F	332	6/6	0.90	0.17	50,52,54,57	0
3	GOL	B	331	6/6	0.91	0.11	54,55,58,64	0
5	EDO	F	570	4/4	0.91	0.12	52,61,64,69	0
3	GOL	B	332	6/6	0.91	0.15	40,49,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	330	6/6	0.91	0.25	43,53,55,57	0
5	EDO	A	346	4/4	0.92	0.25	37,40,41,46	0
3	GOL	A	335	6/6	0.92	0.18	33,44,47,53	0
5	EDO	C	347	4/4	0.92	0.19	37,48,52,52	0
3	GOL	B	330	6/6	0.93	0.17	39,48,53,58	0
3	GOL	C	334	6/6	0.93	0.12	45,55,58,63	0
4	K	E	333	1/1	0.94	0.21	61,61,61,61	0
3	GOL	D	332	6/6	0.94	0.15	40,48,55,60	0
3	GOL	C	332	6/6	0.94	0.18	36,46,58,62	0
3	GOL	B	335	6/6	0.94	0.13	31,38,43,43	0
5	EDO	A	569	4/4	0.94	0.10	47,54,55,59	0
5	EDO	B	339	4/4	0.94	0.28	33,34,35,35	0
3	GOL	E	329	6/6	0.95	0.10	45,46,47,50	0
3	GOL	C	330	6/6	0.95	0.15	41,44,46,49	0
5	EDO	B	346	4/4	0.95	0.33	37,37,42,43	0
5	EDO	D	339	4/4	0.95	0.30	51,55,55,56	0
3	GOL	B	329	6/6	0.95	0.14	31,37,39,43	0
3	GOL	A	329	6/6	0.96	0.09	29,33,34,36	0
5	EDO	C	344	4/4	0.96	0.22	52,55,61,61	0
5	EDO	C	340	4/4	0.96	0.29	35,43,44,44	0
4	K	A	333	1/1	0.96	0.23	50,50,50,50	0
3	GOL	C	329	6/6	0.97	0.09	27,31,31,35	0
4	K	C	333	1/1	0.97	0.17	50,50,50,50	0
4	K	D	333	1/1	0.97	0.15	60,60,60,60	0
5	EDO	F	337	4/4	0.97	0.23	40,43,43,46	0
5	EDO	C	336	4/4	0.98	0.16	28,28,30,30	0
5	EDO	C	339	4/4	0.98	0.25	29,32,34,35	0
4	K	B	333	1/1	0.98	0.15	48,48,48,48	0
5	EDO	A	339	4/4	0.98	0.31	32,33,33,33	0
5	EDO	A	337	4/4	0.98	0.19	26,27,27,30	0
2	PO4	A	328	5/5	0.99	0.07	23,24,25,26	0
2	PO4	E	328	5/5	0.99	0.05	32,34,34,36	0
2	PO4	B	328	5/5	0.99	0.08	21,21,24,24	0
2	PO4	F	328	5/5	0.99	0.06	29,29,34,35	0
2	PO4	C	328	5/5	1.00	0.08	23,23,24,26	0
2	PO4	D	328	5/5	1.00	0.04	30,30,32,35	0

## 6.5 Other polymers

There are no such residues in this entry.