Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 12:32 pm GMT

PDB ID	:	7AJP
Title	:	Crystal Structure of Human Adenovirus 56 Fiber Knob
Authors	:	Strebl, M.; Mindler, K.; Stehle, T.
Deposited on	:	2020-09-29
Resolution	:	1.38 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

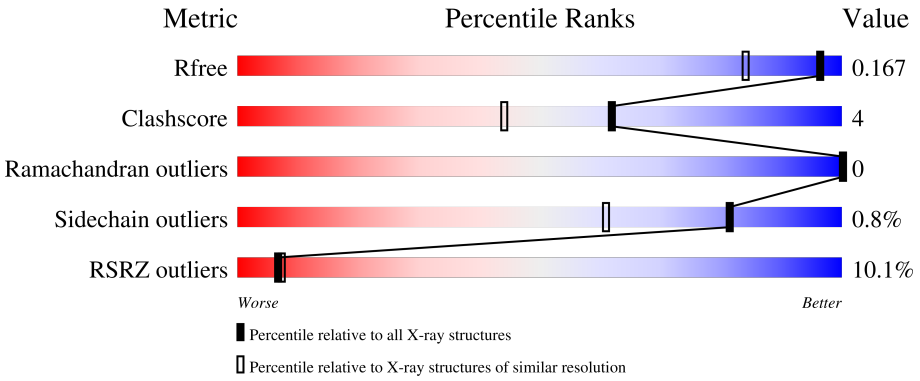
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	208	3% 80% 9% 11%
1	B	208	3% 78% 10% 12%
1	C	208	4% 79% 10% 11%
1	D	208	4% 82% 7% 11%
1	E	208	4% 84% 5% 11%

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Mol	Chain	Length	Quality of chain
1	F	208	7% 81% 6% 13%
1	G	208	7% 80% 9% 12%
1	H	208	9% 82% 6% 12%
1	I	208	6% 81% 9% 11%
1	J	208	21% 83% 6% 11%
1	K	208	23% 83% 7% 11%
1	L	208	18% 85% 12%

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
2	GOL	A	402	-	-	X	-
2	GOL	C	402	-	-	X	-
2	GOL	I	402	-	-	X	-
2	GOL	J	402	-	-	X	-
4	EDO	A	411	-	-	X	-
4	EDO	D	404	-	-	X	-
4	EDO	G	403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20234 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	7	0
			1497	966	233	291	7			
1	B	184	Total	C	N	O	S	0	9	0
			1498	964	237	291	6			
1	C	186	Total	C	N	O	S	0	12	0
			1550	993	248	303	6			
1	D	185	Total	C	N	O	S	0	7	0
			1488	961	236	285	6			
1	E	186	Total	C	N	O	S	0	7	0
			1507	969	237	295	6			
1	F	181	Total	C	N	O	S	0	9	0
			1486	958	235	287	6			
1	G	184	Total	C	N	O	S	0	5	0
			1476	953	232	285	6			
1	H	183	Total	C	N	O	S	0	9	0
			1488	961	237	284	6			
1	I	186	Total	C	N	O	S	0	9	0
			1522	979	240	297	6			
1	J	185	Total	C	N	O	S	0	1	0
			1430	921	226	278	5			
1	K	186	Total	C	N	O	S	0	0	0
			1416	916	223	271	6			
1	L	183	Total	C	N	O	S	0	3	0
			1431	923	225	277	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	MET	-	initiating methionine	UNP R9RU05
A	156	ARG	-	expression tag	UNP R9RU05
A	157	GLY	-	expression tag	UNP R9RU05
A	158	SER	-	expression tag	UNP R9RU05
A	159	HIS	-	expression tag	UNP R9RU05

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Chain	Residue	Modelled	Actual	Comment	Reference
A	160	HIS	-	expression tag	UNP R9RU05
A	161	HIS	-	expression tag	UNP R9RU05
A	162	HIS	-	expression tag	UNP R9RU05
A	163	HIS	-	expression tag	UNP R9RU05
A	164	HIS	-	expression tag	UNP R9RU05
A	165	GLY	-	expression tag	UNP R9RU05
A	166	SER	-	expression tag	UNP R9RU05
B	155	MET	-	initiating methionine	UNP R9RU05
B	156	ARG	-	expression tag	UNP R9RU05
B	157	GLY	-	expression tag	UNP R9RU05
B	158	SER	-	expression tag	UNP R9RU05
B	159	HIS	-	expression tag	UNP R9RU05
B	160	HIS	-	expression tag	UNP R9RU05
B	161	HIS	-	expression tag	UNP R9RU05
B	162	HIS	-	expression tag	UNP R9RU05
B	163	HIS	-	expression tag	UNP R9RU05
B	164	HIS	-	expression tag	UNP R9RU05
B	165	GLY	-	expression tag	UNP R9RU05
B	166	SER	-	expression tag	UNP R9RU05
C	155	MET	-	initiating methionine	UNP R9RU05
C	156	ARG	-	expression tag	UNP R9RU05
C	157	GLY	-	expression tag	UNP R9RU05
C	158	SER	-	expression tag	UNP R9RU05
C	159	HIS	-	expression tag	UNP R9RU05
C	160	HIS	-	expression tag	UNP R9RU05
C	161	HIS	-	expression tag	UNP R9RU05
C	162	HIS	-	expression tag	UNP R9RU05
C	163	HIS	-	expression tag	UNP R9RU05
C	164	HIS	-	expression tag	UNP R9RU05
C	165	GLY	-	expression tag	UNP R9RU05
C	166	SER	-	expression tag	UNP R9RU05
D	155	MET	-	initiating methionine	UNP R9RU05
D	156	ARG	-	expression tag	UNP R9RU05
D	157	GLY	-	expression tag	UNP R9RU05
D	158	SER	-	expression tag	UNP R9RU05
D	159	HIS	-	expression tag	UNP R9RU05
D	160	HIS	-	expression tag	UNP R9RU05
D	161	HIS	-	expression tag	UNP R9RU05
D	162	HIS	-	expression tag	UNP R9RU05
D	163	HIS	-	expression tag	UNP R9RU05
D	164	HIS	-	expression tag	UNP R9RU05
D	165	GLY	-	expression tag	UNP R9RU05

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Chain	Residue	Modelled	Actual	Comment	Reference
D	166	SER	-	expression tag	UNP R9RU05
E	155	MET	-	initiating methionine	UNP R9RU05
E	156	ARG	-	expression tag	UNP R9RU05
E	157	GLY	-	expression tag	UNP R9RU05
E	158	SER	-	expression tag	UNP R9RU05
E	159	HIS	-	expression tag	UNP R9RU05
E	160	HIS	-	expression tag	UNP R9RU05
E	161	HIS	-	expression tag	UNP R9RU05
E	162	HIS	-	expression tag	UNP R9RU05
E	163	HIS	-	expression tag	UNP R9RU05
E	164	HIS	-	expression tag	UNP R9RU05
E	165	GLY	-	expression tag	UNP R9RU05
E	166	SER	-	expression tag	UNP R9RU05
F	155	MET	-	initiating methionine	UNP R9RU05
F	156	ARG	-	expression tag	UNP R9RU05
F	157	GLY	-	expression tag	UNP R9RU05
F	158	SER	-	expression tag	UNP R9RU05
F	159	HIS	-	expression tag	UNP R9RU05
F	160	HIS	-	expression tag	UNP R9RU05
F	161	HIS	-	expression tag	UNP R9RU05
F	162	HIS	-	expression tag	UNP R9RU05
F	163	HIS	-	expression tag	UNP R9RU05
F	164	HIS	-	expression tag	UNP R9RU05
F	165	GLY	-	expression tag	UNP R9RU05
F	166	SER	-	expression tag	UNP R9RU05
G	155	MET	-	initiating methionine	UNP R9RU05
G	156	ARG	-	expression tag	UNP R9RU05
G	157	GLY	-	expression tag	UNP R9RU05
G	158	SER	-	expression tag	UNP R9RU05
G	159	HIS	-	expression tag	UNP R9RU05
G	160	HIS	-	expression tag	UNP R9RU05
G	161	HIS	-	expression tag	UNP R9RU05
G	162	HIS	-	expression tag	UNP R9RU05
G	163	HIS	-	expression tag	UNP R9RU05
G	164	HIS	-	expression tag	UNP R9RU05
G	165	GLY	-	expression tag	UNP R9RU05
G	166	SER	-	expression tag	UNP R9RU05
H	155	MET	-	initiating methionine	UNP R9RU05
H	156	ARG	-	expression tag	UNP R9RU05
H	157	GLY	-	expression tag	UNP R9RU05
H	158	SER	-	expression tag	UNP R9RU05
H	159	HIS	-	expression tag	UNP R9RU05

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Chain	Residue	Modelled	Actual	Comment	Reference
H	160	HIS	-	expression tag	UNP R9RU05
H	161	HIS	-	expression tag	UNP R9RU05
H	162	HIS	-	expression tag	UNP R9RU05
H	163	HIS	-	expression tag	UNP R9RU05
H	164	HIS	-	expression tag	UNP R9RU05
H	165	GLY	-	expression tag	UNP R9RU05
H	166	SER	-	expression tag	UNP R9RU05
I	155	MET	-	initiating methionine	UNP R9RU05
I	156	ARG	-	expression tag	UNP R9RU05
I	157	GLY	-	expression tag	UNP R9RU05
I	158	SER	-	expression tag	UNP R9RU05
I	159	HIS	-	expression tag	UNP R9RU05
I	160	HIS	-	expression tag	UNP R9RU05
I	161	HIS	-	expression tag	UNP R9RU05
I	162	HIS	-	expression tag	UNP R9RU05
I	163	HIS	-	expression tag	UNP R9RU05
I	164	HIS	-	expression tag	UNP R9RU05
I	165	GLY	-	expression tag	UNP R9RU05
I	166	SER	-	expression tag	UNP R9RU05
J	155	MET	-	initiating methionine	UNP R9RU05
J	156	ARG	-	expression tag	UNP R9RU05
J	157	GLY	-	expression tag	UNP R9RU05
J	158	SER	-	expression tag	UNP R9RU05
J	159	HIS	-	expression tag	UNP R9RU05
J	160	HIS	-	expression tag	UNP R9RU05
J	161	HIS	-	expression tag	UNP R9RU05
J	162	HIS	-	expression tag	UNP R9RU05
J	163	HIS	-	expression tag	UNP R9RU05
J	164	HIS	-	expression tag	UNP R9RU05
J	165	GLY	-	expression tag	UNP R9RU05
J	166	SER	-	expression tag	UNP R9RU05
K	155	MET	-	initiating methionine	UNP R9RU05
K	156	ARG	-	expression tag	UNP R9RU05
K	157	GLY	-	expression tag	UNP R9RU05
K	158	SER	-	expression tag	UNP R9RU05
K	159	HIS	-	expression tag	UNP R9RU05
K	160	HIS	-	expression tag	UNP R9RU05
K	161	HIS	-	expression tag	UNP R9RU05
K	162	HIS	-	expression tag	UNP R9RU05
K	163	HIS	-	expression tag	UNP R9RU05
K	164	HIS	-	expression tag	UNP R9RU05
K	165	GLY	-	expression tag	UNP R9RU05

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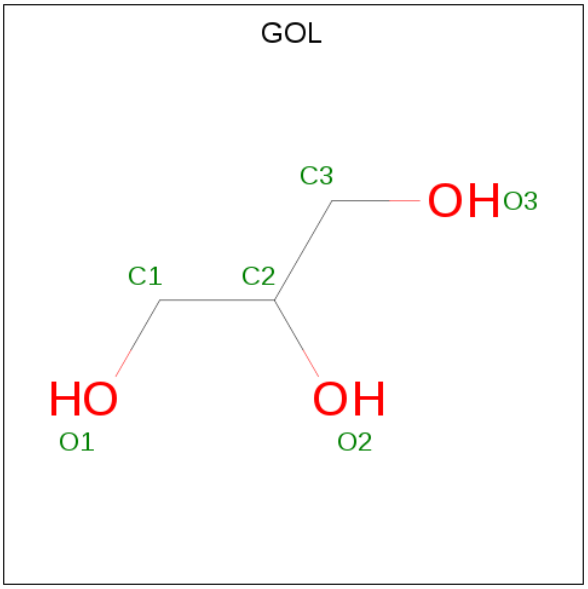
Chain	Residue	Modelled	Actual	Comment	Reference
K	166	SER	-	expression tag	UNP R9RU05
L	155	MET	-	initiating methionine	UNP R9RU05
L	156	ARG	-	expression tag	UNP R9RU05
L	157	GLY	-	expression tag	UNP R9RU05
L	158	SER	-	expression tag	UNP R9RU05
L	159	HIS	-	expression tag	UNP R9RU05
L	160	HIS	-	expression tag	UNP R9RU05
L	161	HIS	-	expression tag	UNP R9RU05
L	162	HIS	-	expression tag	UNP R9RU05
L	163	HIS	-	expression tag	UNP R9RU05
L	164	HIS	-	expression tag	UNP R9RU05
L	165	GLY	-	expression tag	UNP R9RU05
L	166	SER	-	expression tag	UNP R9RU05

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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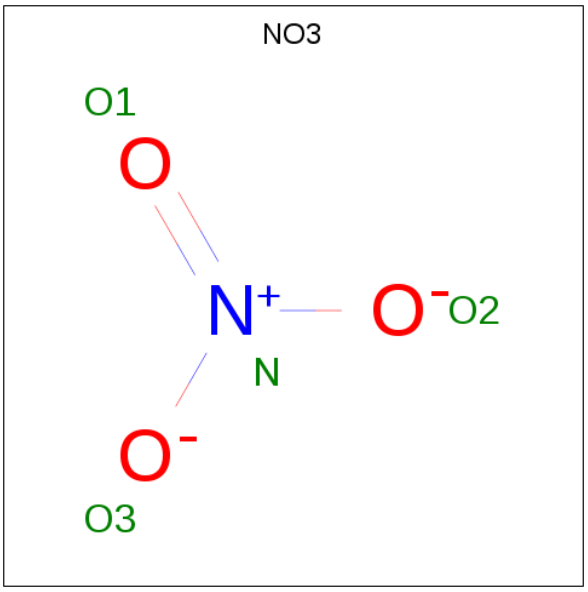
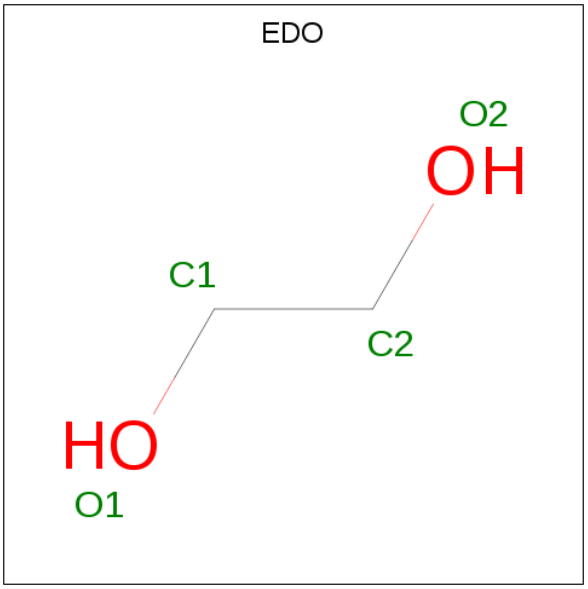
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	D	1	Total N O 4 1 3	0	0
3	E	1	Total N O 4 1 3	0	0
3	E	1	Total N O 4 1 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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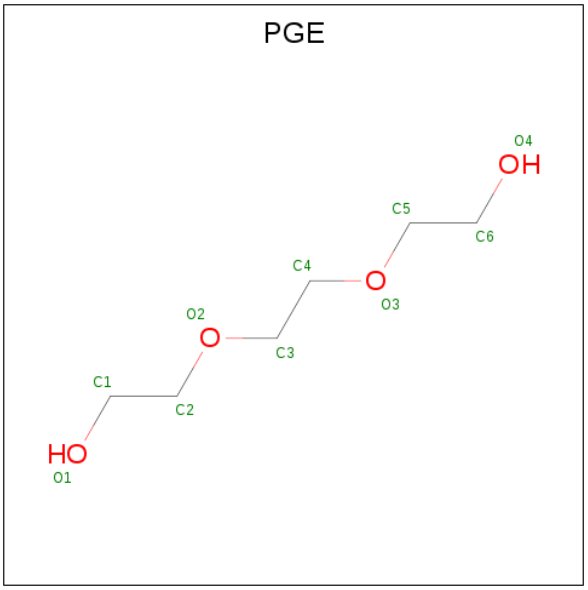
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 7 4 3	0	0
5	L	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

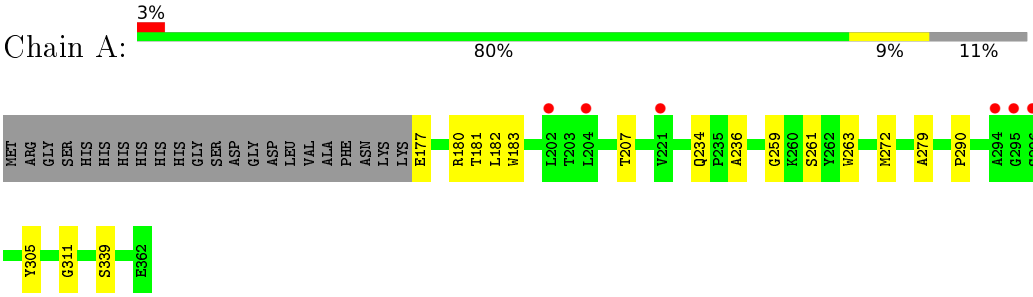
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0
6	B	221	Total O 221 221	0	0
6	C	206	Total O 206 206	0	0
6	D	248	Total O 248 248	0	0
6	E	227	Total O 227 227	0	0
6	F	175	Total O 175 175	0	0
6	G	164	Total O 164 164	0	0
6	H	187	Total O 187 187	0	0
6	I	214	Total O 214 214	0	0
6	J	117	Total O 117 117	0	0
6	K	66	Total O 66 66	0	0
6	L	118	Total O 118 118	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

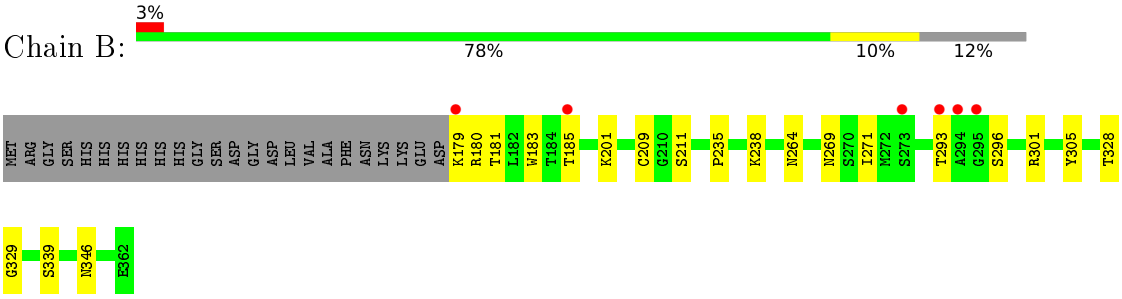
- Molecule 1: Fiber

Chain A:



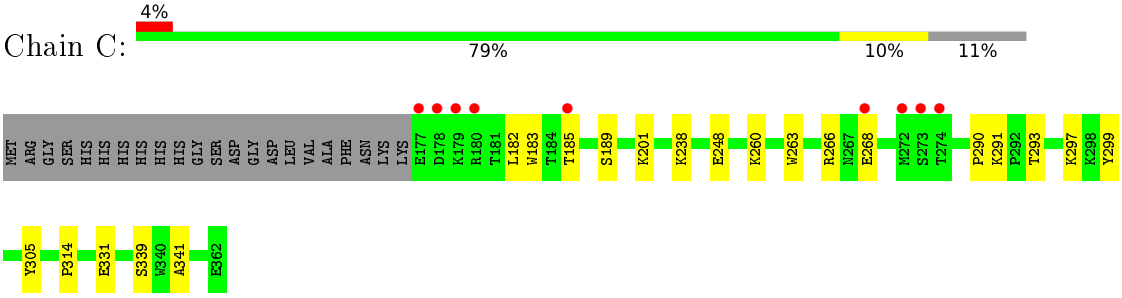
- Molecule 1: Fiber

Chain B:



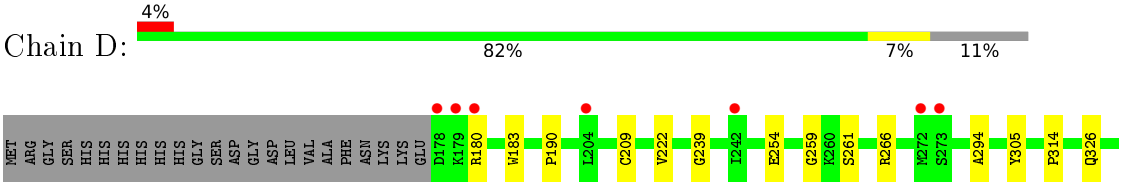
- Molecule 1: Fiber

Chain C:



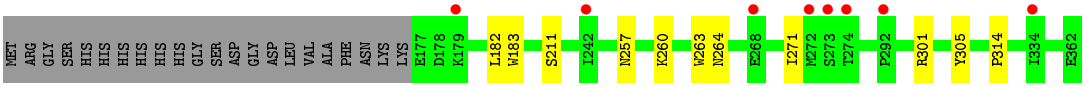
- Molecule 1: Fiber

Chain D:



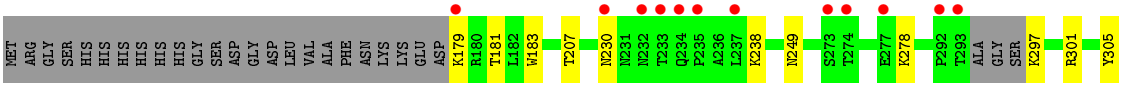
• Molecule 1: Fiber

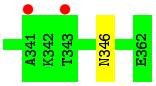
Chain E:



• Molecule 1: Fiber

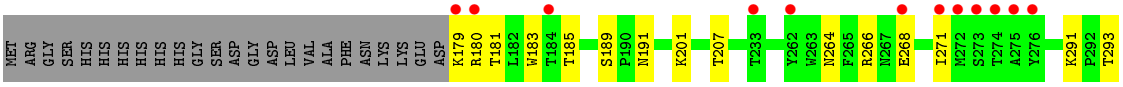
Chain F:

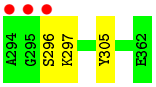




• Molecule 1: Fiber

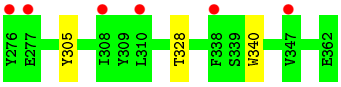
Chain G:





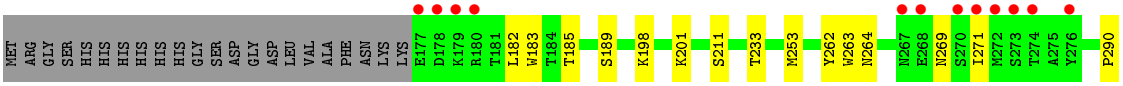
• Molecule 1: Fiber

Chain H:



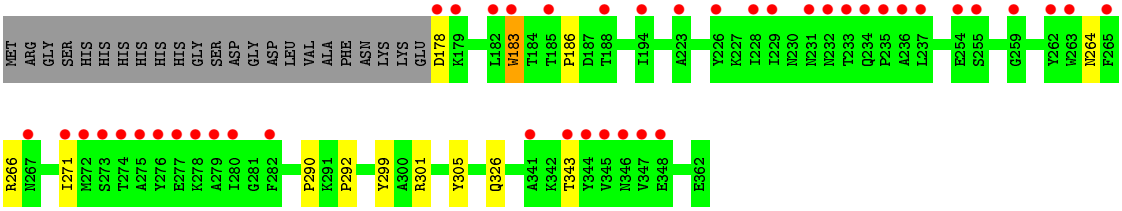
• Molecule 1: Fiber

Chain I:



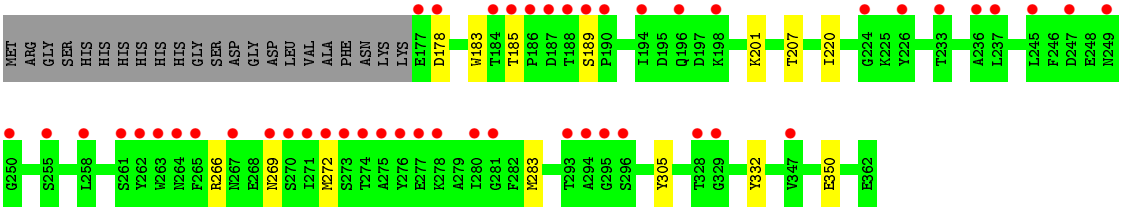
- Molecule 1: Fiber

Chain J:



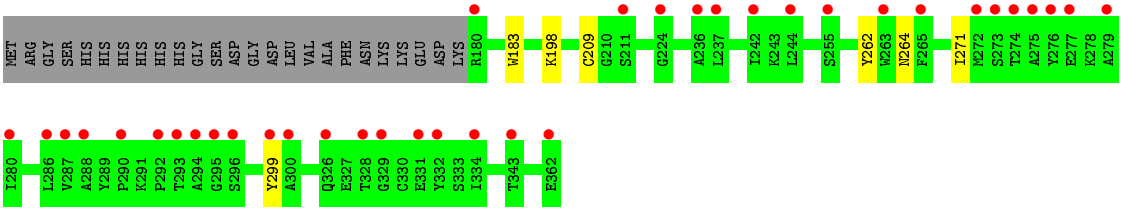
- Molecule 1: Fiber

Chain K:



- Molecule 1: Fiber

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.44Å 182.53Å 117.03Å 90.00° 118.54° 90.00°	Depositor
Resolution (Å)	42.64 – 1.38 49.06 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.64-1.38) 99.0 (49.06-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.38Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.134 , 0.167 0.135 , 0.167	Depositor DCC
R_{free} test set	7366 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	20234	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PGE, EDO, NO3

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	0.55	0/1542	0.75	1/2095 (0.0%)
1	B	0.57	0/1543	0.73	2/2098 (0.1%)
1	C	0.56	0/1598	0.71	0/2166
1	D	0.53	0/1530	0.70	0/2079
1	E	0.57	0/1555	0.73	1/2112 (0.0%)
1	F	0.52	0/1530	0.70	1/2074 (0.0%)
1	G	0.47	0/1521	0.68	0/2064
1	H	0.53	0/1530	0.69	0/2077
1	I	0.51	0/1564	0.67	0/2124
1	J	0.40	0/1463	0.62	0/1992
1	K	0.36	0/1449	0.59	0/1973
1	L	0.38	0/1470	0.58	0/1999
All	All	0.50	0/18295	0.68	5/24853 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	301	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	F	301	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	301	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	301	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	E	301	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1497	0	1480	26	0
1	B	1498	0	1487	17	0
1	C	1550	0	1537	19	0
1	D	1488	0	1476	21	0
1	E	1507	0	1496	9	0
1	F	1486	0	1473	5	0
1	G	1476	0	1471	16	0
1	H	1488	0	1472	9	0
1	I	1522	0	1506	14	0
1	J	1430	0	1369	15	0
1	K	1416	0	1331	10	0
1	L	1431	0	1388	4	0
2	A	12	0	16	9	0
2	B	6	0	8	1	0
2	C	12	0	16	6	0
2	D	6	0	8	1	0
2	E	6	0	8	1	0
2	F	6	0	8	1	0
2	G	12	0	16	1	0
2	H	6	0	8	1	0
2	I	18	0	24	4	0
2	J	12	0	16	10	0
2	K	6	0	8	1	0
2	L	6	0	8	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	D	4	0	0	0	0
3	E	8	0	0	0	0
4	A	32	0	48	13	0
4	B	20	0	30	4	0
4	C	12	0	18	0	0
4	D	16	0	24	12	0
4	E	16	0	24	4	0
4	F	4	0	6	1	0
4	G	4	0	6	5	0
4	H	20	0	30	1	0
4	I	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	4	2	0
5	C	10	0	14	3	0
5	D	4	0	4	1	0
5	E	7	0	9	1	0
5	L	7	0	9	1	0
6	A	210	0	0	1	0
6	B	221	0	0	1	0
6	C	206	0	0	3	0
6	D	248	0	0	2	0
6	E	227	0	0	1	0
6	F	175	0	0	0	0
6	G	164	0	0	2	0
6	H	187	0	0	1	0
6	I	214	0	0	0	0
6	J	117	0	0	0	0
6	K	66	0	0	1	0
6	L	118	0	0	0	0
All	All	20234	0	17868	159	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.

All (159) 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:C:299:TYR:HB2	2:C:402:GOL:H11	1.35	1.06
1:A:301:ARG:HH21	2:A:402:GOL:H11	1.34	0.92
1:I:299:TYR:HD2	2:I:402:GOL:H31	1.39	0.87
1:F:230[B]:ASN:ND2	1:F:346[B]:ASN:OD1	2.08	0.86
1:J:299:TYR:HB2	2:J:402:GOL:H32	1.57	0.85
1:G:191:ASN:HB3	4:G:403:EDO:H11	1.59	0.85
1:A:259:GLY:HA3	4:A:411:EDO:H21	1.58	0.84
1:A:299:TYR:HD2	2:A:402:GOL:H2	1.45	0.81
1:D:261:SER:H	4:D:404:EDO:H11	1.44	0.81
1:I:299:TYR:HB2	2:I:402:GOL:H11	1.63	0.79
1:A:234:GLN:HB3	5:A:412:PGE:H32	1.66	0.78
1:G:189:SER:HG	4:G:403:EDO:HO1	1.26	0.75
1:D:314:PRO:HG3	4:E:405:EDO:H22	1.70	0.73
1:C:339:SER:HB2	5:C:406:PGE:H22	1.70	0.73
1:A:301:ARG:NH2	2:A:402:GOL:H11	2.05	0.71
1:D:294:ALA:HA	4:I:404:EDO:H22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:327:GLU:OE2	1:I:335[B]:THR:HG21	1.91	0.70
1:B:238:LYS:HB3	4:B:404:EDO:H22	1.75	0.69
1:A:290:PRO:CD	2:A:402:GOL:H12	2.24	0.68
1:A:259:GLY:CA	4:A:411:EDO:H21	2.26	0.66
1:D:259:GLY:HA3	4:D:404:EDO:H12	1.77	0.66
4:A:409:EDO:H11	6:A:564:HOH:O	1.95	0.65
1:I:299:TYR:CD2	2:I:402:GOL:H31	2.28	0.65
1:A:290:PRO:HG2	2:A:402:GOL:H32	1.80	0.64
1:C:266[A]:ARG:NE	1:C:268:GLU:O	2.27	0.64
1:B:339:SER:HB2	4:B:404:EDO:H21	1.80	0.63
1:J:301:ARG:NH2	2:J:402:GOL:H31	2.14	0.63
1:B:185[B]:THR:O	1:B:201:LYS:NZ	2.30	0.63
1:J:264:ASN:HB3	1:J:271:ILE:HB	1.81	0.63
1:B:185[A]:THR:O	1:B:201:LYS:NZ	2.23	0.62
1:E:314:PRO:HG3	4:F:402:EDO:H12	1.82	0.62
1:H:305:TYR:HB3	2:H:401:GOL:H32	1.82	0.62
1:B:235:PRO:HB2	5:L:402:PGE:H6	1.82	0.61
1:C:182[A]:LEU:HG	1:C:263:TRP:CZ2	2.35	0.61
1:I:253:MET:HA	4:I:405:EDO:H11	1.83	0.61
1:A:261:SER:H	4:A:411:EDO:H22	1.67	0.60
1:H:328:THR:HA	4:H:404:EDO:H11	1.83	0.60
1:D:261:SER:H	4:D:404:EDO:C1	2.13	0.59
4:A:404:EDO:H22	4:A:409:EDO:H21	1.84	0.59
1:D:261:SER:HB2	4:D:404:EDO:H11	1.85	0.58
1:H:269:ASN:ND2	6:H:501:HOH:O	2.32	0.58
1:I:182[B]:LEU:HG	1:I:263:TRP:CZ2	2.39	0.58
1:A:290:PRO:HD3	2:A:402:GOL:H12	1.85	0.57
1:D:266:ARG:HD3	1:E:211[A]:SER:OG	2.05	0.57
1:H:238[B]:LYS:NZ	1:H:340:TRP:O	2.38	0.57
1:A:261:SER:HB2	4:A:411:EDO:H22	1.87	0.56
1:E:305:TYR:HB3	2:E:401:GOL:H32	1.87	0.56
1:F:179:LYS:HD3	1:F:181:THR:H	1.70	0.56
1:K:220:ILE:HD13	1:K:350:GLU:HB2	1.87	0.56
1:A:177:GLU:HA	1:A:272[B]:MET:SD	2.45	0.56
1:D:254:GLU:H	4:D:403:EDO:H21	1.70	0.56
1:J:301:ARG:HH21	2:J:402:GOL:H31	1.70	0.56
1:E:305:TYR:OH	4:E:405:EDO:H21	2.04	0.56
1:B:305:TYR:HB3	2:B:401:GOL:H11	1.87	0.56
4:B:403:EDO:H12	1:C:297:LYS:NZ	2.21	0.55
1:D:239:GLY:O	4:D:406:EDO:H11	2.06	0.55
1:G:179:LYS:HD3	1:G:181:THR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:SER:HB3	4:A:409:EDO:H12	1.88	0.55
1:F:305:TYR:HB3	2:F:401:GOL:H32	1.89	0.54
1:J:290:PRO:CD	2:J:402:GOL:H2	2.37	0.54
1:D:261:SER:CB	4:D:404:EDO:H11	2.37	0.54
1:I:185:THR:HG23	1:I:269:ASN:O	2.08	0.54
1:C:299:TYR:CD2	2:C:402:GOL:H31	2.43	0.53
1:A:261:SER:H	4:A:411:EDO:C2	2.22	0.53
1:C:299:TYR:HD2	2:C:402:GOL:H31	1.74	0.53
1:D:326:GLN:NE2	6:D:504:HOH:O	2.42	0.53
1:C:305:TYR:HB3	2:C:401:GOL:H11	1.90	0.53
1:B:179:LYS:HE2	1:B:180:ARG:H	1.74	0.53
1:G:291:LYS:NZ	6:G:501:HOH:O	2.36	0.52
1:J:299:TYR:CD2	2:J:402:GOL:H12	2.44	0.52
1:G:264:ASN:HB3	1:G:271:ILE:HB	1.90	0.52
1:J:305:TYR:HB3	2:J:401:GOL:H11	1.91	0.52
1:G:179:LYS:HD3	1:G:180:ARG:N	2.25	0.52
1:I:198:LYS:NZ	1:I:262:TYR:OH	2.43	0.52
4:D:404:EDO:H21	6:D:680:HOH:O	2.11	0.51
1:D:254:GLU:H	4:D:403:EDO:C2	2.23	0.51
1:G:185:THR:O	1:G:201:LYS:NZ	2.38	0.51
1:B:328[B]:THR:HG23	6:B:541:HOH:O	2.11	0.50
1:D:261:SER:N	4:D:404:EDO:H11	2.22	0.50
1:J:290:PRO:HD2	2:J:402:GOL:H2	1.94	0.50
1:J:178:ASP:HB3	1:J:266:ARG:HB3	1.93	0.50
1:C:189[B]:SER:O	1:C:201:LYS:HD3	2.11	0.50
1:H:264:ASN:HB3	1:H:271:ILE:HB	1.93	0.50
1:C:238:LYS:HB3	5:C:406:PGE:H2	1.93	0.50
1:G:179:LYS:HD3	1:G:180:ARG:H	1.77	0.50
1:J:299:TYR:HD2	2:J:402:GOL:H12	1.76	0.50
1:D:314:PRO:CG	4:E:405:EDO:H22	2.41	0.49
1:E:264:ASN:HB3	1:E:271:ILE:HB	1.95	0.48
1:B:346[B]:ASN:ND2	4:B:407:EDO:O1	2.39	0.48
1:A:299:TYR:CD2	2:A:402:GOL:H2	2.37	0.48
1:A:305:TYR:HB3	2:A:401:GOL:H11	1.94	0.48
1:D:266:ARG:HH11	1:E:211[A]:SER:HB3	1.79	0.48
1:E:257:ASN:O	4:E:404:EDO:H11	2.14	0.48
1:D:259:GLY:CA	4:D:404:EDO:H12	2.42	0.48
1:A:279:ALA:HA	4:A:405:EDO:H12	1.96	0.48
1:G:305:TYR:HB3	2:G:401:GOL:H32	1.94	0.48
1:K:305:TYR:HB3	2:K:401:GOL:H32	1.96	0.48
1:A:259:GLY:C	4:A:411:EDO:H21	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:THR:HB	1:B:296:SER:HB2	1.95	0.47
1:I:189[A]:SER:O	1:I:201:LYS:HD3	2.13	0.47
1:A:182[A]:LEU:HG	1:A:263:TRP:CZ2	2.49	0.47
1:B:328[A]:THR:HG22	1:B:329:GLY:N	2.29	0.47
1:E:182[B]:LEU:HG	1:E:263:TRP:CZ2	2.49	0.47
1:K:220:ILE:HD12	1:L:299:TYR:CD1	2.50	0.47
4:A:404:EDO:H21	1:C:314:PRO:HG3	1.97	0.46
1:H:266:ARG:HD3	1:I:211[A]:SER:OG	2.15	0.46
1:G:297[A]:LYS:NZ	6:G:503:HOH:O	2.39	0.46
1:L:198:LYS:NZ	1:L:262:TYR:OH	2.44	0.46
1:G:201:LYS:HZ2	4:G:403:EDO:C2	2.29	0.45
1:G:189:SER:OG	4:G:403:EDO:O1	2.15	0.45
1:C:290:PRO:CD	2:C:402:GOL:H2	2.47	0.45
1:A:261:SER:CB	4:A:411:EDO:H22	2.46	0.45
1:D:305:TYR:HB3	2:D:401:GOL:H11	1.98	0.45
1:C:260:LYS:HB2	6:C:648:HOH:O	2.16	0.45
1:K:185:THR:HG23	1:K:269:ASN:O	2.17	0.45
1:A:311:GLY:O	4:A:408:EDO:H11	2.16	0.45
1:C:185:THR:HG21	6:C:556:HOH:O	2.16	0.45
1:C:293[B]:THR:HG21	6:C:661:HOH:O	2.16	0.45
1:H:189:SER:O	1:H:201[B]:LYS:HD3	2.16	0.45
1:I:264:ASN:HB3	1:I:271:ILE:HB	1.99	0.45
1:A:180:ARG:O	1:A:180:ARG:HG2	2.17	0.45
1:B:185[A]:THR:HG23	1:B:269:ASN:O	2.17	0.45
5:E:408:PGE:H52	5:E:408:PGE:H3	1.68	0.44
1:G:266:ARG:NE	1:G:268:GLU:O	2.44	0.44
1:G:293:THR:OG1	1:G:296:SER:HB3	2.17	0.44
1:F:249:ASN:OD1	1:F:278:LYS:HE3	2.17	0.44
1:K:207:THR:HG21	1:L:209:CYS:O	2.18	0.44
1:J:299:TYR:H	2:J:402:GOL:C1	2.31	0.44
1:D:190:PRO:HG3	1:D:222:VAL:HG21	2.00	0.44
1:D:209:CYS:O	1:F:207:THR:HG21	2.18	0.43
1:B:328[A]:THR:HG22	1:B:329:GLY:H	1.82	0.43
1:J:299:TYR:H	2:J:402:GOL:H12	1.84	0.43
1:B:179:LYS:HG3	1:B:181:THR:H	1.83	0.43
1:A:236:ALA:HB3	5:A:412:PGE:H3	1.99	0.42
1:D:180:ARG:HH21	5:D:407:PGE:H4	1.83	0.42
1:K:272:MET:HE2	1:K:272:MET:HA	2.01	0.42
1:I:233:THR:HA	1:J:343:THR:OG1	2.19	0.42
1:A:181:THR:OG1	1:B:211[A]:SER:OG	2.07	0.42
1:L:264:ASN:HB3	1:L:271:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:292:PRO:HD3	1:J:326:GLN:OE1	2.20	0.42
1:A:290:PRO:HD2	2:A:402:GOL:H12	1.99	0.42
1:B:264:ASN:HB3	1:B:271:ILE:HB	2.01	0.42
1:C:290:PRO:CG	2:C:402:GOL:H2	2.49	0.42
1:C:341:ALA:HB2	5:C:406:PGE:H42	2.02	0.42
1:C:248[A]:GLU:HB3	1:C:331[A]:GLU:HG3	2.01	0.41
1:K:189:SER:O	1:K:201:LYS:HD3	2.20	0.41
1:D:259:GLY:C	4:D:404:EDO:H12	2.40	0.41
1:K:283:MET:HB3	1:K:332:TYR:CD1	2.55	0.41
1:G:207:THR:HG21	1:H:209:CYS:O	2.21	0.41
1:C:291:LYS:O	1:C:293[B]:THR:HG23	2.20	0.41
1:G:189:SER:O	4:G:403:EDO:H12	2.21	0.41
1:I:189[B]:SER:O	1:I:201:LYS:HD3	2.20	0.41
1:A:207:THR:HG21	1:B:209:CYS:O	2.20	0.41
1:K:220:ILE:HD11	6:K:517:HOH:O	2.19	0.41
1:I:290:PRO:HD2	2:I:402:GOL:H2	2.03	0.40
1:J:183:TRP:CH2	1:J:186:PRO:HD3	2.56	0.40
1:H:238[B]:LYS:HA	1:H:238[B]:LYS:HD2	1.98	0.40
1:K:178:ASP:HB3	1:K:266:ARG:HB3	2.04	0.40
1:E:260:LYS:HB2	6:E:664:HOH:O	2.21	0.40

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	191/208 (92%)	183 (96%)	8 (4%)	0	100	100
1	B	191/208 (92%)	185 (97%)	6 (3%)	0	100	100
1	C	196/208 (94%)	189 (96%)	7 (4%)	0	100	100
1	D	190/208 (91%)	182 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	192/208 (92%)	184 (96%)	8 (4%)	0	100	100
1	F	186/208 (89%)	181 (97%)	5 (3%)	0	100	100
1	G	187/208 (90%)	181 (97%)	6 (3%)	0	100	100
1	H	190/208 (91%)	184 (97%)	6 (3%)	0	100	100
1	I	193/208 (93%)	186 (96%)	7 (4%)	0	100	100
1	J	184/208 (88%)	176 (96%)	8 (4%)	0	100	100
1	K	184/208 (88%)	175 (95%)	9 (5%)	0	100	100
1	L	184/208 (88%)	176 (96%)	8 (4%)	0	100	100
All	All	2268/2496 (91%)	2182 (96%)	86 (4%)	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	167/183 (91%)	166 (99%)	1 (1%)	86	70
1	B	168/183 (92%)	167 (99%)	1 (1%)	86	70
1	C	175/183 (96%)	174 (99%)	1 (1%)	86	70
1	D	165/183 (90%)	164 (99%)	1 (1%)	86	70
1	E	171/183 (93%)	170 (99%)	1 (1%)	86	70
1	F	168/183 (92%)	165 (98%)	3 (2%)	59	27
1	G	165/183 (90%)	164 (99%)	1 (1%)	86	70
1	H	164/183 (90%)	162 (99%)	2 (1%)	71	45
1	I	171/183 (93%)	170 (99%)	1 (1%)	86	70
1	J	152/183 (83%)	151 (99%)	1 (1%)	84	65
1	K	142/183 (78%)	141 (99%)	1 (1%)	84	65
1	L	154/183 (84%)	153 (99%)	1 (1%)	86	70
All	All	1962/2196 (89%)	1947 (99%)	15 (1%)	81	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	TRP
1	B	183	TRP
1	C	183	TRP
1	D	183	TRP
1	E	183	TRP
1	F	183	TRP
1	F	238	LYS
1	F	297	LYS
1	G	183	TRP
1	H	183	TRP
1	H	197	ASP
1	I	183	TRP
1	J	183	TRP
1	K	183	TRP
1	L	183	TRP

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

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 monosaccharides in this entry.

5.6 Ligand geometry

61 ligands are modelled in this entry.

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

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^{th} 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^2)	Q<0.9
1	A	186/208 (89%)	0.50	6 (3%) 47 49	13, 17, 30, 52	3 (1%)
1	B	184/208 (88%)	0.34	6 (3%) 46 48	13, 19, 40, 50	0
1	C	186/208 (89%)	0.40	9 (4%) 30 32	13, 18, 30, 45	0
1	D	185/208 (88%)	0.50	8 (4%) 35 37	13, 18, 34, 62	0
1	E	186/208 (89%)	0.57	8 (4%) 35 37	13, 17, 30, 42	0
1	F	181/208 (87%)	0.46	14 (7%) 13 14	14, 21, 37, 51	0
1	G	184/208 (88%)	0.58	15 (8%) 11 11	16, 26, 45, 61	0
1	H	183/208 (87%)	0.72	18 (9%) 7 8	14, 19, 36, 57	0
1	I	186/208 (89%)	0.48	12 (6%) 18 19	14, 20, 35, 52	0
1	J	185/208 (88%)	1.22	43 (23%) 0 0	20, 32, 58, 69	0
1	K	186/208 (89%)	1.55	48 (25%) 0 0	27, 44, 61, 71	0
1	L	183/208 (87%)	1.21	37 (20%) 1 0	20, 35, 53, 78	0
All	All	2215/2496 (88%)	0.71	224 (10%) 7 7	13, 22, 50, 78	3 (0%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	294	ALA	9.0
1	L	295	GLY	8.2
1	H	273	SER	7.9
1	J	262	TYR	7.6
1	K	185	THR	7.3
1	J	275	ALA	7.2
1	J	274	THR	7.0
1	L	293	THR	6.9
1	L	299	TYR	6.8
1	K	237	LEU	6.6
1	K	272	MET	6.2

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Mol	Chain	Res	Type	RSRZ
1	K	294	ALA	5.7
1	K	275	ALA	5.7
1	I	273	SER	5.5
1	J	273	SER	5.5
1	J	272	MET	5.4
1	L	328	THR	5.4
1	K	262	TYR	5.2
1	H	274	THR	5.2
1	L	274	THR	5.1
1	L	296	SER	4.9
1	L	292	PRO	4.9
1	K	265	PHE	4.9
1	K	276	TYR	4.9
1	K	273	SER	4.8
1	G	273	SER	4.8
1	K	329	GLY	4.7
1	K	271	ILE	4.7
1	J	276	TYR	4.6
1	K	274	THR	4.6
1	K	236	ALA	4.6
1	E	273	SER	4.5
1	J	233	THR	4.4
1	H	275	ALA	4.4
1	I	274	THR	4.3
1	K	278	LYS	4.2
1	K	255	SER	4.2
1	G	272	MET	4.1
1	J	277	GLU	4.1
1	J	179	LYS	4.0
1	F	235	PRO	4.0
1	K	196	GLN	4.0
1	L	276	TYR	3.9
1	G	268	GLU	3.9
1	B	294	ALA	3.8
1	L	275	ALA	3.8
1	K	281	GLY	3.8
1	K	263	TRP	3.8
1	H	276	TYR	3.8
1	I	272	MET	3.8
1	D	178	ASP	3.7
1	K	190	PRO	3.7
1	G	271	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	224	GLY	3.7
1	J	188	THR	3.7
1	K	226	TYR	3.6
1	B	273	SER	3.6
1	H	277	GLU	3.6
1	J	343	THR	3.6
1	K	187	ASP	3.6
1	B	293	THR	3.6
1	I	177	GLU	3.6
1	H	229[A]	ILE	3.5
1	K	249	ASN	3.5
1	K	269	ASN	3.5
1	J	226	TYR	3.5
1	H	272	MET	3.5
1	C	274	THR	3.5
1	G	179	LYS	3.5
1	I	179	LYS	3.5
1	K	270	SER	3.5
1	A	294	ALA	3.4
1	J	232	ASN	3.4
1	A	296	SER	3.4
1	J	229	ILE	3.4
1	K	188	THR	3.4
1	J	237	LEU	3.4
1	J	345	VAL	3.3
1	J	341	ALA	3.3
1	J	185	THR	3.3
1	C	179	LYS	3.3
1	I	271	ILE	3.3
1	L	279	ALA	3.3
1	C	177	GLU	3.3
1	L	236	ALA	3.2
1	L	290	PRO	3.2
1	H	271	ILE	3.2
1	F	237	LEU	3.2
1	K	245	LEU	3.1
1	L	263	TRP	3.1
1	G	295	GLY	3.1
1	J	235	PRO	3.1
1	J	223	ALA	3.1
1	F	343	THR	3.1
1	J	228	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	347	VAL	3.1
1	D	272	MET	3.0
1	K	178	ASP	3.0
1	L	286	LEU	3.0
1	G	262	TYR	3.0
1	B	179	LYS	3.0
1	H	220	ILE	3.0
1	J	271	ILE	3.0
1	L	277	GLU	3.0
1	J	347	VAL	3.0
1	K	184	THR	3.0
1	J	263	TRP	2.9
1	L	242	ILE	2.9
1	L	280	ILE	2.9
1	L	265	PHE	2.9
1	G	275	ALA	2.9
1	D	179	LYS	2.9
1	L	273	SER	2.9
1	J	194	ILE	2.9
1	K	177	GLU	2.8
1	L	343	THR	2.8
1	F	234	GLN	2.8
1	F	232	ASN	2.8
1	I	180	ARG	2.8
1	L	287	VAL	2.8
1	I	178	ASP	2.8
1	I	276	TYR	2.8
1	L	332	TYR	2.8
1	L	180	ARG	2.8
1	L	326	GLN	2.7
1	K	186	PRO	2.7
1	G	276	TYR	2.7
1	G	184	THR	2.7
1	K	261	SER	2.7
1	F	293	THR	2.7
1	K	250	GLY	2.7
1	K	233	THR	2.7
1	D	180	ARG	2.7
1	H	217	VAL	2.7
1	K	194	ILE	2.6
1	L	237	LEU	2.6
1	J	254	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	262	TYR	2.6
1	K	258	LEU	2.6
1	C	178	ASP	2.6
1	F	292	PRO	2.6
1	L	272	MET	2.6
1	J	259	GLY	2.5
1	L	362	GLU	2.5
1	H	310	LEU	2.5
1	K	198	LYS	2.5
1	G	274	THR	2.5
1	G	296	SER	2.5
1	A	204	LEU	2.5
1	J	178	ASP	2.5
1	K	264	ASN	2.5
1	J	344	TYR	2.5
1	J	346	ASN	2.4
1	K	247	ASP	2.4
1	I	268	GLU	2.4
1	F	233	THR	2.4
1	C	268	GLU	2.4
1	E	268	GLU	2.4
1	D	273	SER	2.4
1	L	211	SER	2.4
1	K	267	ASN	2.4
1	K	277	GLU	2.4
1	G	294	ALA	2.3
1	H	308	ILE	2.3
1	K	328	THR	2.3
1	G	180	ARG	2.3
1	K	295	GLY	2.3
1	F	341	ALA	2.3
1	F	179	LYS	2.3
1	J	255	SER	2.3
1	K	189	SER	2.3
1	H	267	ASN	2.3
1	H	269	ASN	2.3
1	E	242	ILE	2.3
1	J	182	LEU	2.3
1	J	234	GLN	2.3
1	L	300	ALA	2.3
1	K	347	VAL	2.3
1	J	267	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	280	ILE	2.2
1	K	224	GLY	2.2
1	F	273[A]	SER	2.2
1	F	274	THR	2.2
1	F	230[A]	ASN	2.2
1	K	280	ILE	2.2
1	J	279	ALA	2.2
1	K	293	THR	2.2
1	C	273[A]	SER	2.2
1	J	183	TRP	2.2
1	J	236	ALA	2.2
1	C	180	ARG	2.2
1	L	331	GLU	2.1
1	J	265	PHE	2.1
1	L	329	GLY	2.1
1	E	179	LYS	2.1
1	F	277	GLU	2.1
1	K	296	SER	2.1
1	B	185[A]	THR	2.1
1	J	278	LYS	2.1
1	H	338	PHE	2.1
1	L	288	ALA	2.1
1	J	231	ASN	2.1
1	D	204	LEU	2.1
1	B	295	GLY	2.1
1	C	185	THR	2.1
1	D	242	ILE	2.1
1	E	292	PRO	2.1
1	L	255	SER	2.1
1	A	295	GLY	2.1
1	C	272	MET	2.1
1	E	274	THR	2.1
1	I	267	ASN	2.1
1	J	348	GLU	2.1
1	I	270	SER	2.1
1	A	221	VAL	2.1
1	L	334	ILE	2.1
1	A	202	LEU	2.0
1	E	272	MET	2.0
1	D	334	ILE	2.0
1	E	334	ILE	2.0
1	G	233[A]	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	282	PHE	2.0
1	H	219	LEU	2.0
1	L	244	LEU	2.0

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
5	PGE	E	408	7/10	0.50	0.27	73,74,75,75	0
4	EDO	B	403	4/4	0.58	0.24	60,61,61,62	0
4	EDO	C	404	4/4	0.66	0.23	48,50,52,54	0
4	EDO	H	404	4/4	0.67	0.21	57,58,59,60	0
4	EDO	A	406	4/4	0.69	0.25	62,63,63,63	0
5	PGE	C	406	10/10	0.69	0.25	58,63,64,64	0
4	EDO	B	404	4/4	0.70	0.26	59,61,62,64	0
4	EDO	A	407	4/4	0.72	0.15	57,57,57,57	0
2	GOL	I	403	6/6	0.72	0.20	49,53,55,57	0
4	EDO	B	405	4/4	0.74	0.35	58,59,60,61	0
4	EDO	C	405	4/4	0.74	0.21	71,72,73,73	0
5	PGE	A	412	4/10	0.76	0.17	45,48,51,52	0
4	EDO	H	406	4/4	0.76	0.15	59,60,60,60	0
4	EDO	E	407	4/4	0.76	0.20	67,68,69,70	0
4	EDO	A	409	4/4	0.77	0.26	53,54,55,55	0
3	NO3	B	402	4/4	0.77	0.17	51,52,53,53	4
4	EDO	E	406	4/4	0.77	0.20	49,50,51,51	0
4	EDO	A	408	4/4	0.78	0.15	48,50,51,53	0
2	GOL	G	402	6/6	0.79	0.18	41,47,48,50	0
4	EDO	B	406	4/4	0.80	0.19	64,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	H	402	4/4	0.80	0.19	62,62,62,63	0
4	EDO	H	403	4/4	0.81	0.20	58,60,61,61	0
4	EDO	C	403	4/4	0.81	0.14	46,47,47,47	0
4	EDO	I	405	4/4	0.83	0.19	56,57,58,58	0
4	EDO	G	403	4/4	0.83	0.25	77,77,77,77	0
4	EDO	D	406	4/4	0.84	0.21	63,65,66,66	0
4	EDO	F	402	4/4	0.84	0.20	53,56,57,58	0
4	EDO	D	405	4/4	0.85	0.11	59,59,59,60	0
4	EDO	H	405	4/4	0.85	0.24	66,67,68,68	0
4	EDO	A	404	4/4	0.85	0.18	54,56,57,58	0
4	EDO	E	404	4/4	0.86	0.15	46,47,48,49	0
2	GOL	L	401	6/6	0.86	0.12	44,45,47,48	0
4	EDO	D	404	4/4	0.87	0.20	28,36,39,43	0
5	PGE	L	402	7/10	0.87	0.18	42,50,53,53	0
4	EDO	B	407	4/4	0.88	0.14	74,75,75,75	0
3	NO3	D	402	4/4	0.89	0.12	73,73,74,74	0
2	GOL	J	401	6/6	0.90	0.11	42,43,44,47	0
2	GOL	A	402	6/6	0.90	0.18	45,48,51,54	0
5	PGE	D	407	4/10	0.90	0.24	52,54,56,56	0
2	GOL	B	401	6/6	0.90	0.10	31,35,37,40	0
4	EDO	I	404	4/4	0.90	0.18	56,59,61,63	0
2	GOL	J	402	6/6	0.90	0.19	38,41,42,46	0
2	GOL	K	401	6/6	0.91	0.09	50,51,52,53	0
3	NO3	A	403	4/4	0.91	0.17	73,74,75,75	0
4	EDO	A	410	4/4	0.92	0.14	28,34,38,40	0
4	EDO	A	411	4/4	0.92	0.15	21,30,31,37	0
2	GOL	C	402	6/6	0.92	0.18	22,25,28,30	6
4	EDO	A	405	4/4	0.92	0.15	46,47,47,48	0
2	GOL	I	402	6/6	0.92	0.24	28,33,34,35	6
2	GOL	D	401	6/6	0.92	0.08	34,35,37,39	0
2	GOL	E	401	6/6	0.92	0.09	30,32,36,38	0
2	GOL	A	401	6/6	0.93	0.09	31,33,34,37	0
2	GOL	H	401	6/6	0.93	0.14	33,36,37,38	0
2	GOL	C	401	6/6	0.94	0.09	29,32,34,36	0
4	EDO	D	403	4/4	0.94	0.23	49,50,51,53	0
2	GOL	I	401	6/6	0.94	0.12	36,38,39,42	0
2	GOL	F	401	6/6	0.94	0.10	35,35,36,39	0
4	EDO	E	405	4/4	0.94	0.14	33,34,38,39	0
2	GOL	G	401	6/6	0.94	0.09	38,39,40,43	0
3	NO3	E	402	4/4	0.95	0.20	56,56,57,59	0
3	NO3	E	403	4/4	0.97	0.10	16,23,24,25	4

6.5 Other polymers (i)

There are no such residues in this entry.