wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 04:34 PM EDT

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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

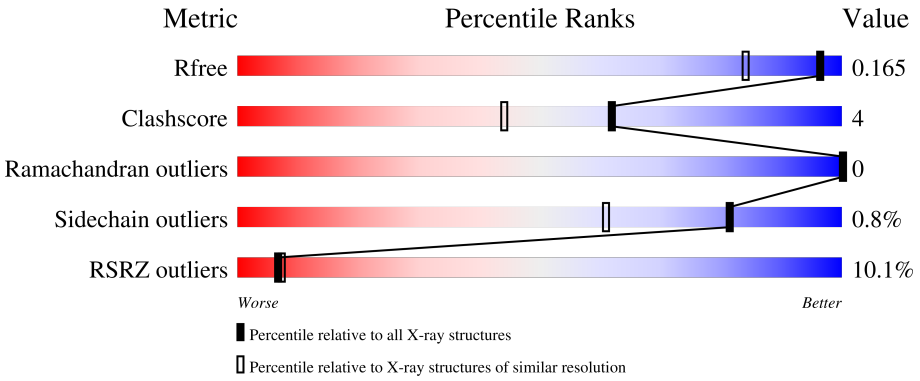
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 (i)

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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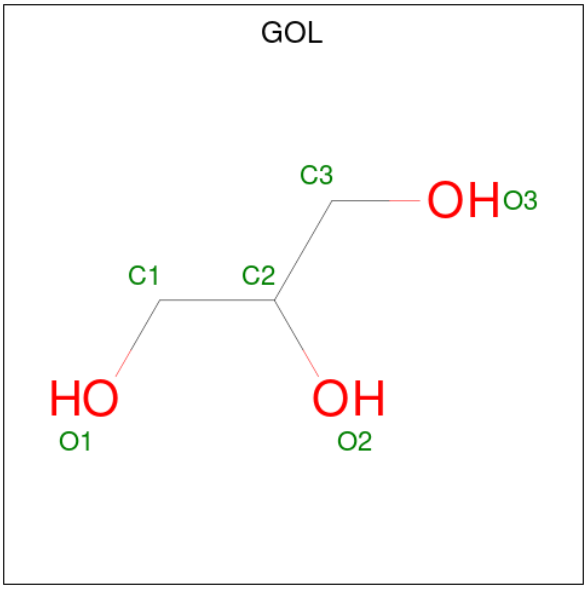
Chain	Residue	Modelled	Actual	Comment	Reference
K	166	SER	-	expression tag	UNP R9RU05
L	155	MET	-	initiating methionine	UNP R9RU05
L	156	ARG	-	expression tag	UNP R9RU05
L	157	GLY	-	expression tag	UNP R9RU05
L	158	SER	-	expression tag	UNP R9RU05
L	159	HIS	-	expression tag	UNP R9RU05
L	160	HIS	-	expression 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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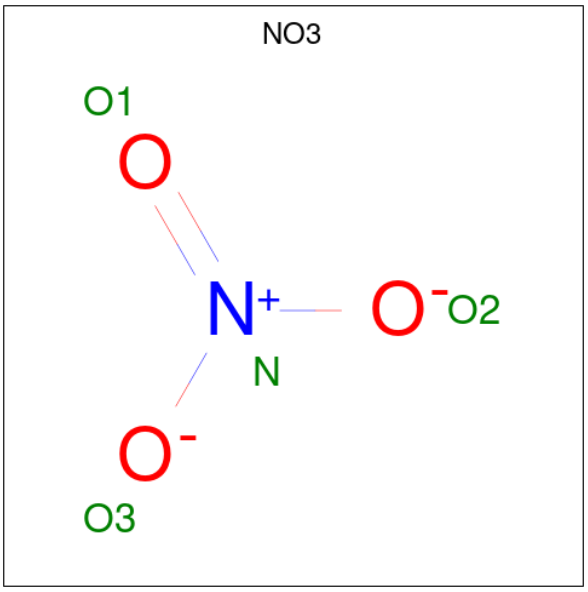
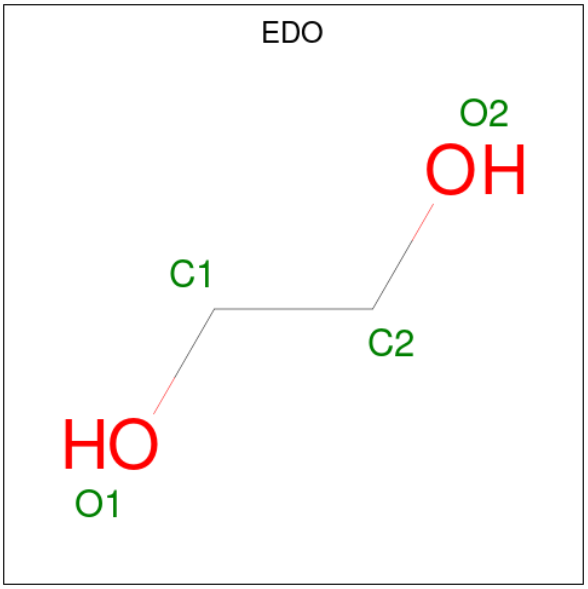
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	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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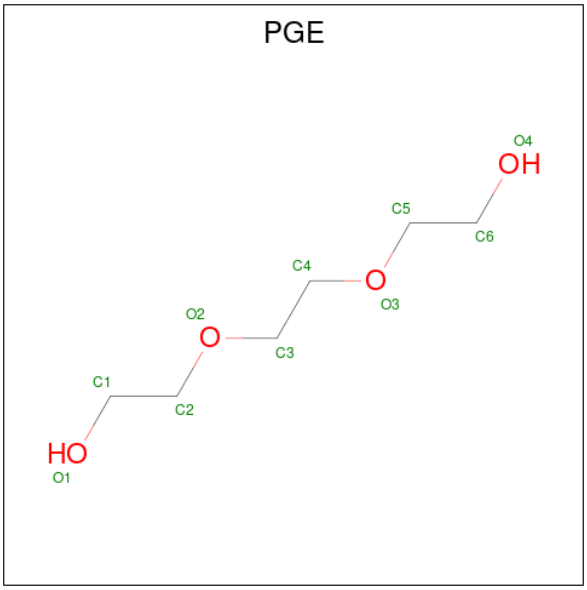
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
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.

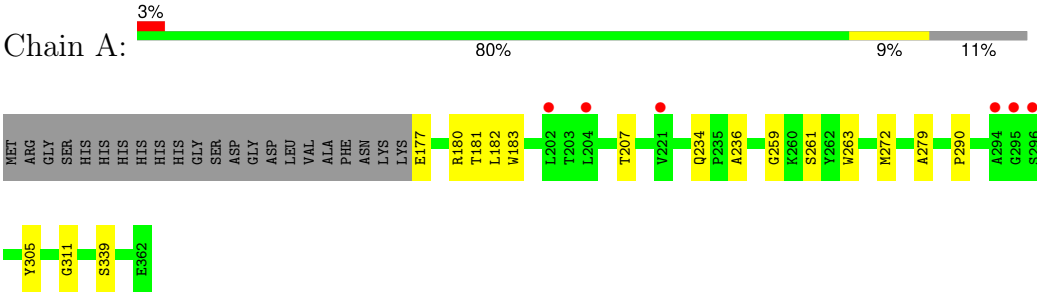
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0
6	B	221	Total O 221 221	0	0
6	C	206	Total O 206 206	0	0
6	D	248	Total O 248 248	0	0
6	E	227	Total O 227 227	0	0
6	F	175	Total O 175 175	0	0
6	G	164	Total O 164 164	0	0
6	H	187	Total O 187 187	0	0
6	I	214	Total O 214 214	0	0
6	J	117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

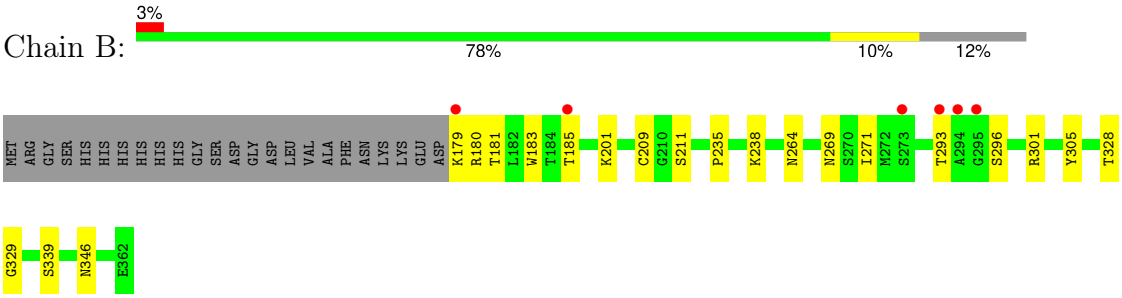
• Molecule 1: Fiber

Chain A:



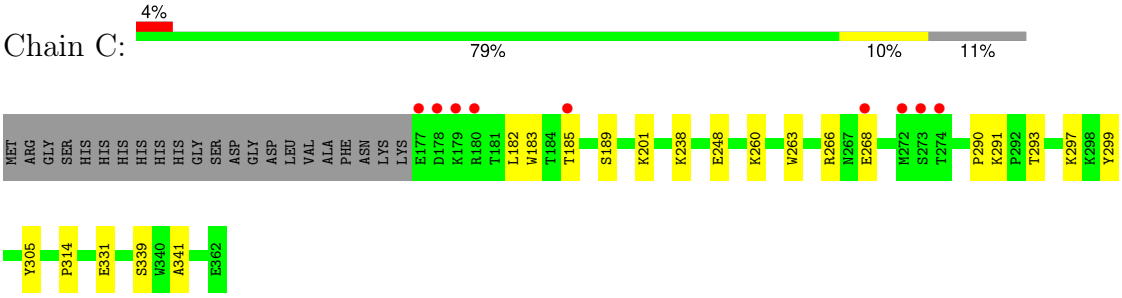
• Molecule 1: Fiber

Chain B:



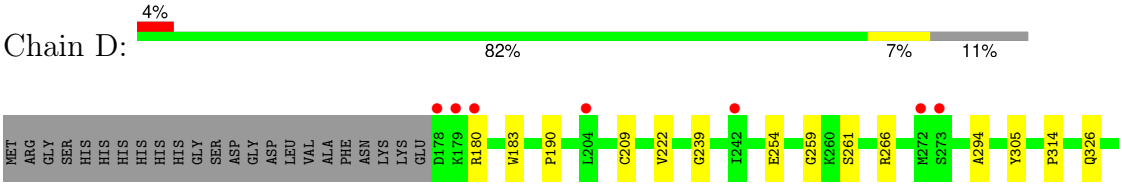
• Molecule 1: Fiber

Chain C:



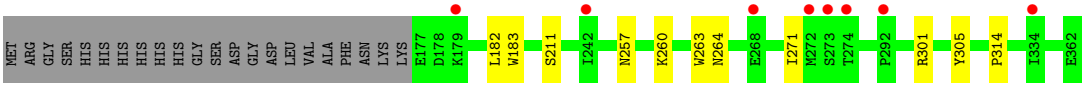
• Molecule 1: Fiber

Chain D:



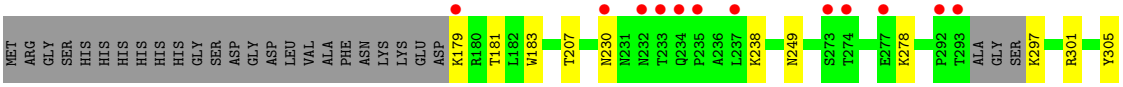
• Molecule 1: Fiber

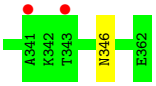
Chain E:



• Molecule 1: Fiber

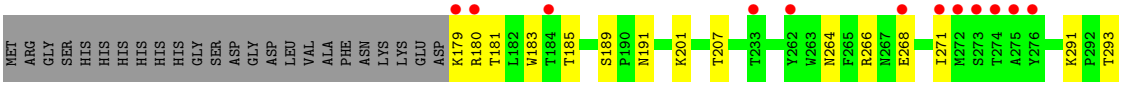
Chain F:

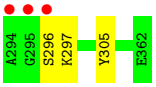




• Molecule 1: Fiber

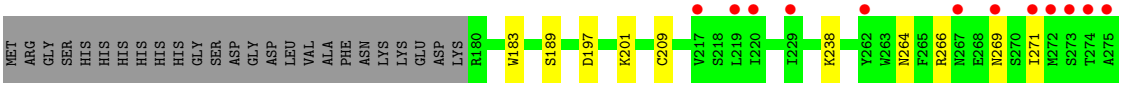
Chain G:

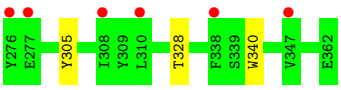




• Molecule 1: Fiber

Chain H:



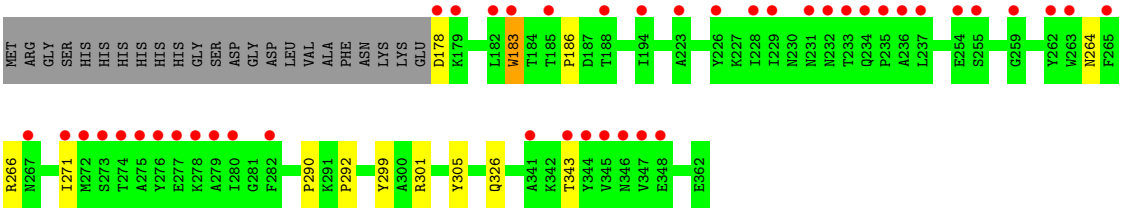


• Molecule 1: Fiber

Chain I:

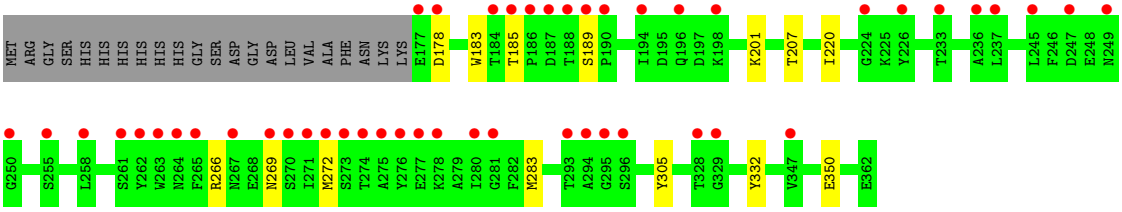
• Molecule 1: Fiber

Chain J:



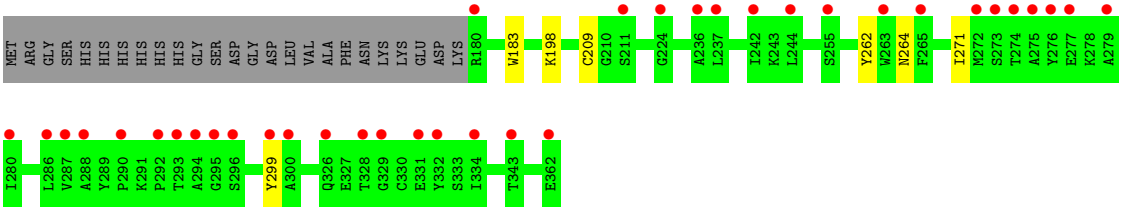
• Molecule 1: Fiber

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 0.134 , 0.165	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: NO3, PGE, GOL, 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	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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	297	LYS
1	K	183	TRP
1	G	183	TRP
1	L	183	TRP
1	I	183	TRP

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

61 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NO3	A	403	-	1,3,3	0.48	0	0,3,3	-	-
4	EDO	B	403	-	3,3,3	0.48	0	2,2,2	0.19	0
4	EDO	G	403	-	3,3,3	0.30	0	2,2,2	0.41	0
2	GOL	A	402	-	5,5,5	0.61	0	5,5,5	1.03	0
2	GOL	I	403	-	5,5,5	0.38	0	5,5,5	0.50	0
3	NO3	B	402	-	1,3,3	0.62	0	0,3,3	-	-
4	EDO	A	405	-	3,3,3	0.34	0	2,2,2	0.50	0
4	EDO	E	406	-	3,3,3	0.47	0	2,2,2	0.23	0
2	GOL	D	401	-	5,5,5	0.48	0	5,5,5	0.85	0
2	GOL	C	401	-	5,5,5	0.42	0	5,5,5	0.88	0
3	NO3	D	402	-	1,3,3	0.55	0	0,3,3	-	-
4	EDO	H	405	-	3,3,3	0.46	0	2,2,2	0.27	0
2	GOL	E	401	-	5,5,5	0.43	0	5,5,5	1.01	0
4	EDO	H	403	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	H	406	-	3,3,3	0.41	0	2,2,2	0.58	0
2	GOL	J	401	-	5,5,5	0.38	0	5,5,5	0.44	0
4	EDO	A	410	-	3,3,3	0.44	0	2,2,2	0.15	0
4	EDO	A	406	-	3,3,3	0.54	0	2,2,2	0.07	0
4	EDO	E	407	-	3,3,3	0.43	0	2,2,2	0.43	0
4	EDO	A	407	-	3,3,3	0.44	0	2,2,2	0.43	0
2	GOL	C	402	-	5,5,5	1.13	0	5,5,5	0.86	0
4	EDO	A	409	-	3,3,3	0.52	0	2,2,2	0.29	0
2	GOL	I	401	-	5,5,5	0.38	0	5,5,5	0.71	0
4	EDO	C	404	-	3,3,3	0.60	0	2,2,2	0.10	0
2	GOL	K	401	-	5,5,5	0.45	0	5,5,5	0.53	0
4	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.30	0
3	NO3	E	402	-	1,3,3	0.69	0	0,3,3	-	-
4	EDO	D	405	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	H	402	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	D	406	-	3,3,3	0.42	0	2,2,2	0.29	0
5	PGE	C	406	-	9,9,9	0.32	0	8,8,8	0.39	0
2	GOL	I	402	-	5,5,5	0.79	0	5,5,5	0.48	0
4	EDO	D	404	-	3,3,3	0.32	0	2,2,2	0.71	0
4	EDO	E	404	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	E	405	-	3,3,3	0.33	0	2,2,2	0.92	0
4	EDO	A	411	-	3,3,3	0.26	0	2,2,2	1.67	1 (50%)
2	GOL	G	402	-	5,5,5	0.42	0	5,5,5	0.69	0
2	GOL	G	401	-	5,5,5	0.38	0	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	C	405	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	I	404	-	3,3,3	0.40	0	2,2,2	0.37	0
5	PGE	A	412	-	3,3,9	0.31	0	2,2,8	0.42	0
5	PGE	D	407	-	3,3,9	0.29	0	2,2,8	0.44	0
2	GOL	L	401	-	5,5,5	0.34	0	5,5,5	0.58	0
4	EDO	I	405	-	3,3,3	0.42	0	2,2,2	0.35	0
5	PGE	L	402	-	6,6,9	0.35	0	5,5,8	0.37	0
4	EDO	A	404	-	3,3,3	0.45	0	2,2,2	0.06	0
5	PGE	E	408	-	6,6,9	0.34	0	5,5,8	0.29	0
4	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.36	0
2	GOL	F	401	-	5,5,5	0.44	0	5,5,5	0.71	0
4	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	F	402	-	3,3,3	0.49	0	2,2,2	0.11	0
2	GOL	H	401	-	5,5,5	0.36	0	5,5,5	0.81	0
4	EDO	A	408	-	3,3,3	0.41	0	2,2,2	0.49	0
4	EDO	B	406	-	3,3,3	0.38	0	2,2,2	0.51	0
3	NO3	E	403	-	1,3,3	0.49	0	0,3,3	-	-
4	EDO	D	403	-	3,3,3	0.34	0	2,2,2	0.51	0
2	GOL	B	401	-	5,5,5	0.40	0	5,5,5	0.81	0
2	GOL	J	402	-	5,5,5	0.64	0	5,5,5	0.57	0
2	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.57	0
4	EDO	H	404	-	3,3,3	0.47	0	2,2,2	0.24	0
4	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.09	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
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	G	403	-	-	0/1/1/1	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	I	403	-	-	2/4/4/4	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	E	406	-	-	1/1/1/1	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
4	EDO	H	405	-	-	0/1/1/1	-
2	GOL	E	401	-	-	2/4/4/4	-
4	EDO	H	403	-	-	1/1/1/1	-
4	EDO	H	406	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	J	401	-	-	2/4/4/4	-
4	EDO	A	410	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	E	407	-	-	1/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
2	GOL	C	402	-	-	4/4/4/4	-
4	EDO	A	409	-	-	1/1/1/1	-
2	GOL	I	401	-	-	2/4/4/4	-
4	EDO	C	404	-	-	1/1/1/1	-
2	GOL	K	401	-	-	0/4/4/4	-
4	EDO	B	404	-	-	1/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	H	402	-	-	0/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
5	PGE	C	406	-	-	3/7/7/7	-
2	GOL	I	402	-	-	4/4/4/4	-
4	EDO	D	404	-	-	1/1/1/1	-
4	EDO	E	404	-	-	1/1/1/1	-
4	EDO	E	405	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
2	GOL	G	402	-	-	2/4/4/4	-
2	GOL	G	401	-	-	2/4/4/4	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	I	404	-	-	1/1/1/1	-
5	PGE	A	412	-	-	0/1/1/7	-
5	PGE	D	407	-	-	1/1/1/7	-
2	GOL	L	401	-	-	2/4/4/4	-
4	EDO	I	405	-	-	0/1/1/1	-
5	PGE	L	402	-	-	4/4/4/7	-
4	EDO	A	404	-	-	1/1/1/1	-
5	PGE	E	408	-	-	3/4/4/7	-
4	EDO	B	405	-	-	1/1/1/1	-
2	GOL	F	401	-	-	2/4/4/4	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	F	402	-	-	1/1/1/1	-
2	GOL	H	401	-	-	2/4/4/4	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	J	402	-	-	3/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
4	EDO	H	404	-	-	1/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	411	EDO	O1-C1-C2	-2.15	96.05	112.39

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	C	402	GOL	O1-C1-C2-O2
2	C	402	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-C3

There are no ring outliers.

37 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	EDO	1	0
4	G	403	EDO	5	0
2	A	402	GOL	8	0
4	A	405	EDO	1	0
2	D	401	GOL	1	0
2	C	401	GOL	1	0
2	E	401	GOL	1	0
2	J	401	GOL	1	0
2	C	402	GOL	5	0
4	A	409	EDO	3	0
2	K	401	GOL	1	0
4	B	404	EDO	2	0
4	D	406	EDO	1	0
5	C	406	PGE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	402	GOL	4	0
4	D	404	EDO	9	0
4	E	404	EDO	1	0
4	E	405	EDO	3	0
4	A	411	EDO	7	0
2	G	401	GOL	1	0
4	I	404	EDO	1	0
5	A	412	PGE	2	0
5	D	407	PGE	1	0
4	I	405	EDO	1	0
5	L	402	PGE	1	0
4	A	404	EDO	2	0
5	E	408	PGE	1	0
2	F	401	GOL	1	0
4	F	402	EDO	1	0
2	H	401	GOL	1	0
4	A	408	EDO	1	0
4	D	403	EDO	2	0
2	B	401	GOL	1	0
2	J	402	GOL	9	0
2	A	401	GOL	1	0
4	H	404	EDO	1	0
4	B	407	EDO	1	0

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%)

The worst 5 of 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

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 (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
5	PGE	C	406	10/10	0.69	0.25	58,63,64,64	0
4	EDO	A	406	4/4	0.69	0.25	62,63,63,63	0
4	EDO	B	404	4/4	0.70	0.26	59,61,62,64	0
2	GOL	I	403	6/6	0.72	0.20	49,53,55,57	0
4	EDO	A	407	4/4	0.72	0.15	57,57,57,57	0
4	EDO	C	405	4/4	0.74	0.21	71,72,73,73	0
4	EDO	B	405	4/4	0.74	0.35	58,59,60,61	0
5	PGE	A	412	4/10	0.76	0.17	45,48,51,52	0
4	EDO	E	407	4/4	0.76	0.20	67,68,69,70	0
4	EDO	H	406	4/4	0.76	0.15	59,60,60,60	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	H	402	4/4	0.80	0.19	62,62,62,63	0
4	EDO	B	406	4/4	0.80	0.19	64,65,66,67	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	F	402	4/4	0.84	0.20	53,56,57,58	0
4	EDO	D	406	4/4	0.84	0.21	63,65,66,66	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	D	405	4/4	0.85	0.11	59,59,59,60	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	B	401	6/6	0.90	0.10	31,35,37,40	0
2	GOL	J	401	6/6	0.90	0.11	42,43,44,47	0
2	GOL	J	402	6/6	0.90	0.19	38,41,42,46	0
5	PGE	D	407	4/10	0.90	0.24	52,54,56,56	0
2	GOL	A	402	6/6	0.90	0.18	45,48,51,54	0
4	EDO	I	404	4/4	0.90	0.18	56,59,61,63	0
3	NO3	A	403	4/4	0.91	0.17	73,74,75,75	0
2	GOL	K	401	6/6	0.91	0.09	50,51,52,53	0
4	EDO	A	405	4/4	0.92	0.15	46,47,47,48	0
2	GOL	E	401	6/6	0.92	0.09	30,32,36,38	0
2	GOL	C	402	6/6	0.92	0.18	22,25,28,30	6
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
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	H	401	6/6	0.93	0.14	33,36,37,38	0
2	GOL	A	401	6/6	0.93	0.09	31,33,34,37	0
2	GOL	G	401	6/6	0.94	0.09	38,39,40,43	0
4	EDO	E	405	4/4	0.94	0.14	33,34,38,39	0
4	EDO	D	403	4/4	0.94	0.23	49,50,51,53	0
2	GOL	C	401	6/6	0.94	0.09	29,32,34,36	0
2	GOL	F	401	6/6	0.94	0.10	35,35,36,39	0
2	GOL	I	401	6/6	0.94	0.12	36,38,39,42	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.