



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2016 – 09:17 PM EDT

PDB ID : 5E24
Title : Structure of the Su(H)-Hairless-DNA Repressor Complex
Authors : Kovall, R.A.; Yuan, Z.
Deposited on : 2015-09-30
Resolution : 2.14 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

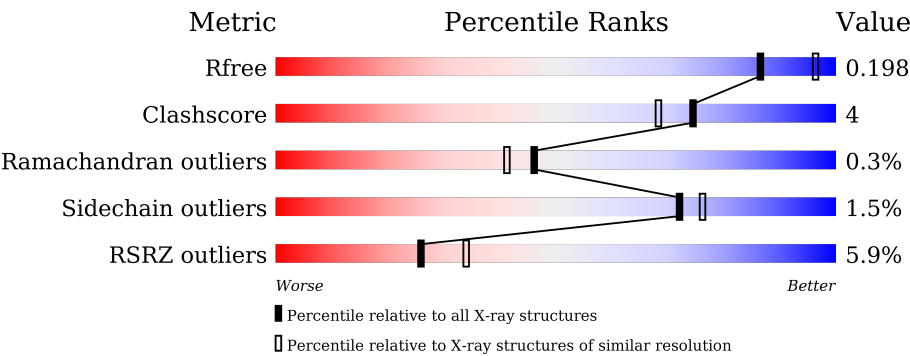
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




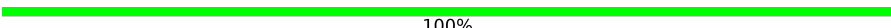
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	<div><div></div><div>92%8%</div></div>
1	C	370	<div><div>5%</div><div>94%6%</div></div>
2	B	38	<div><div>18%</div><div>79%21%</div></div>
2	D	38	<div><div>16%</div><div>76%21%</div><div>.</div></div>
3	E	424	<div><div>5%</div><div>92%7%</div></div>
3	F	424	<div><div>11%</div><div>89%10%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	15	 87% 13%
5	H	15	 100%

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
6	EDO	A	401	-	-	-	X
6	EDO	A	403	-	-	-	X
6	EDO	A	407	-	-	-	X
6	EDO	A	408	-	-	-	X
6	EDO	A	411	-	-	-	X
6	EDO	A	412	-	-	-	X
6	EDO	A	414	-	-	-	X
6	EDO	A	416	-	-	-	X
6	EDO	A	420	-	-	-	X
6	EDO	A	421	-	-	-	X
6	EDO	A	424	-	-	-	X
6	EDO	A	425	-	-	-	X
6	EDO	A	426	-	-	-	X
6	EDO	A	428	-	-	-	X
6	EDO	A	429	-	-	-	X
6	EDO	A	430	-	-	-	X
6	EDO	A	431	-	-	-	X
6	EDO	A	432	-	-	-	X
6	EDO	A	433	-	-	-	X
6	EDO	A	434	-	-	-	X
6	EDO	A	436	-	-	-	X
6	EDO	A	437	-	-	-	X
6	EDO	A	438	-	-	-	X
6	EDO	A	441	-	-	-	X
6	EDO	A	442	-	-	-	X
6	EDO	A	443	-	-	-	X
6	EDO	A	446	-	-	-	X
6	EDO	A	448	-	-	-	X
6	EDO	C	401	-	-	-	X
6	EDO	C	403	-	-	-	X
6	EDO	C	404	-	-	-	X
6	EDO	C	405	-	-	-	X
6	EDO	C	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	C	408	-	-	-	X
6	EDO	C	409	-	-	-	X
6	EDO	C	412	-	-	-	X
6	EDO	E	605	-	-	-	X
6	EDO	E	608	-	-	-	X
6	EDO	E	610	-	-	-	X
6	EDO	E	612	-	-	-	X
6	EDO	E	616	-	-	-	X
6	EDO	E	617	-	-	-	X
6	EDO	E	619	-	-	-	X
6	EDO	E	621	-	-	-	X
6	EDO	E	622	-	-	-	X
6	EDO	E	623	-	-	X	X
6	EDO	E	624	-	-	-	X
6	EDO	F	605	-	-	-	X
6	EDO	F	607	-	-	-	X
6	EDO	F	609	-	-	-	X
6	EDO	F	610	-	-	-	X
6	EDO	F	611	-	-	-	X
6	EDO	F	613	-	-	-	X
6	EDO	F	614	-	-	-	X
6	EDO	F	617	-	-	-	X
6	EDO	F	618	-	-	-	X
6	EDO	F	622	-	-	-	X
6	EDO	F	623	-	-	-	X
6	EDO	F	624	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14968 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	5	0
			2876	1849	470	551	6			
1	C	370	Total	C	N	O	S	0	2	0
			2851	1835	466	544	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	engineered mutation	UNP P0AEY0
A	83	ALA	LYS	engineered mutation	UNP P0AEY0
A	172	ALA	GLU	engineered mutation	UNP P0AEY0
A	173	ALA	ASN	engineered mutation	UNP P0AEY0
A	239	ALA	LYS	engineered mutation	UNP P0AEY0
A	367	ASN	ARG	engineered mutation	UNP P0AEY0
C	82	ALA	ASP	engineered mutation	UNP P0AEY0
C	83	ALA	LYS	engineered mutation	UNP P0AEY0
C	172	ALA	GLU	engineered mutation	UNP P0AEY0
C	173	ALA	ASN	engineered mutation	UNP P0AEY0
C	239	ALA	LYS	engineered mutation	UNP P0AEY0
C	367	ASN	ARG	engineered mutation	UNP P0AEY0

- Molecule 2 is a protein called Protein hairless.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	38	Total	C	N	O	0	0	0
			292	189	55	48			
2	D	38	Total	C	N	O	0	0	0
			292	189	55	48			

- Molecule 3 is a protein called Suppressor of hairless protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	424	Total	C	N	O	S	0	11	0
			3445	2180	595	641	29			
3	F	422	Total	C	N	O	S	0	5	0
			3392	2146	583	634	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	155	THR	ARG	engineered mutation	UNP P28159
E	281	GLY	ASN	engineered mutation	UNP P28159
F	155	THR	ARG	engineered mutation	UNP P28159
F	281	GLY	ASN	engineered mutation	UNP P28159

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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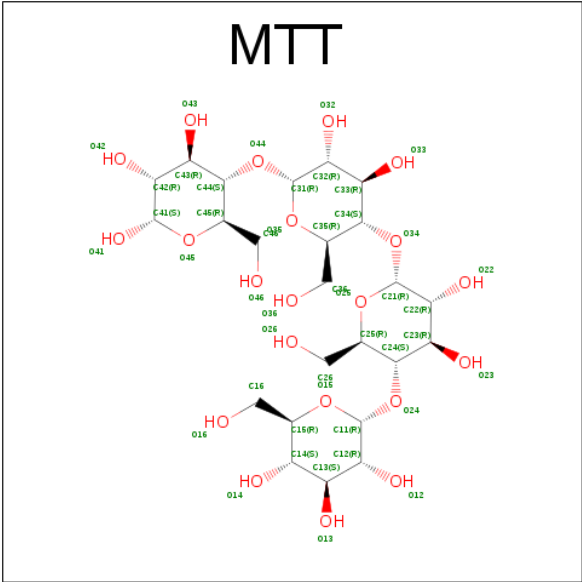
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is MALTOTETRAOSE (three-letter code: MTT) (formula: C₂₄H₄₂O₂₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			45	24	21		
7	C	1	Total	C	O	0	0
			45	24	21		

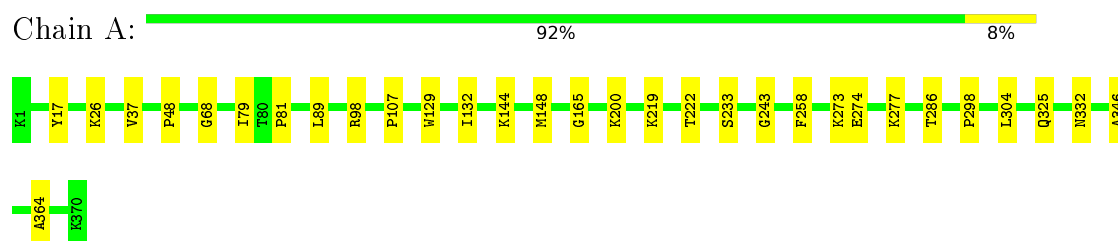
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	283	Total	O	0	0
			283	283		
8	B	8	Total	O	0	0
			8	8		
8	C	96	Total	O	0	0
			96	96		
8	D	9	Total	O	0	0
			9	9		
8	E	174	Total	O	0	0
			174	174		
8	F	80	Total	O	0	0
			80	80		
8	G	6	Total	O	0	0
			6	6		
8	H	13	Total	O	0	0
			13	13		

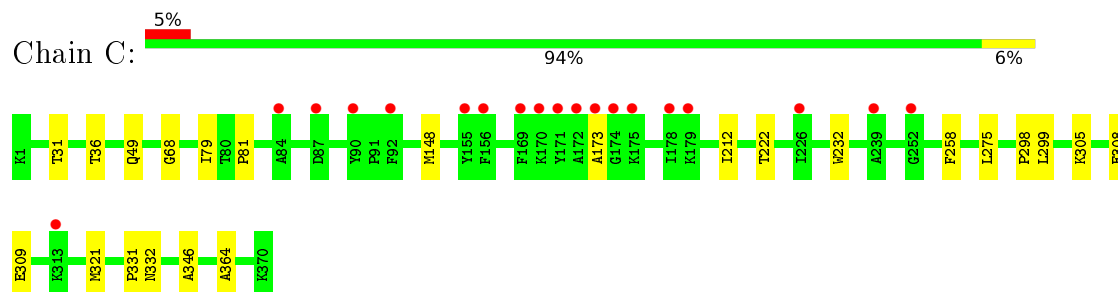
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

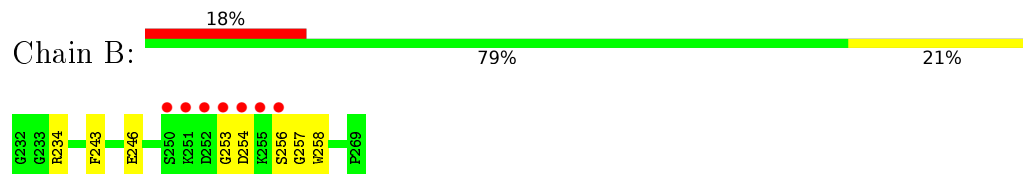
- Molecule 1: Maltose-binding periplasmic protein



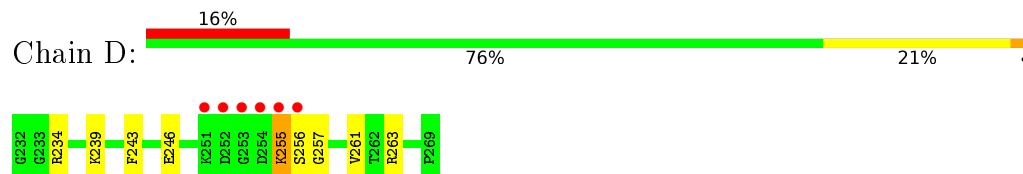
- Molecule 1: Maltose-binding periplasmic protein



- Molecule 2: Protein hairless

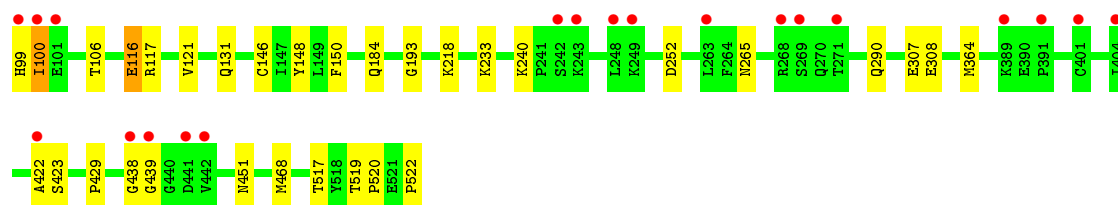


- Molecule 2: Protein hairless

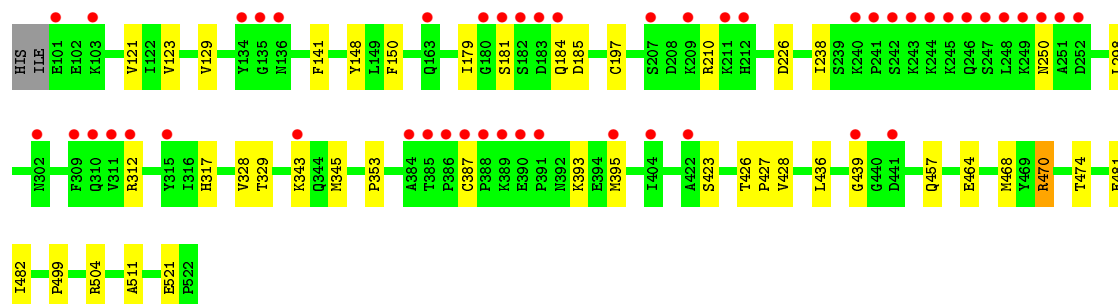
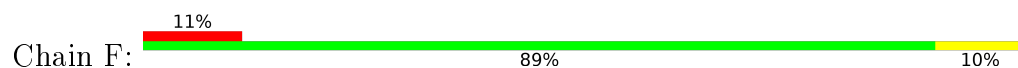


- Molecule 3: Suppressor of hairless protein

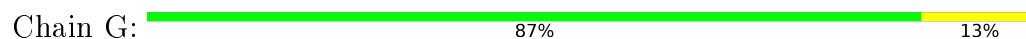




• Molecule 3: Suppressor of hairless protein



• Molecule 4: DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3')



• Molecule 5: DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.71Å 93.89Å 154.39Å 90.00° 109.83° 90.00°	Depositor
Resolution (Å)	31.30 – 2.14 31.32 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.30-2.14) 100.0 (31.32-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.173 , 0.193 0.175 , 0.198	Depositor DCC
R_{free} test set	6594 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14968	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.57	0/2945	0.59	0/4004
1	C	0.48	0/2920	0.59	0/3971
2	B	0.46	0/299	0.69	0/400
2	D	0.49	0/299	0.77	1/400 (0.2%)
3	E	0.47	0/3525	0.63	0/4763
3	F	0.45	0/3467	0.64	0/4684
4	G	1.11	0/332	0.97	0/509
5	H	1.11	0/350	0.91	0/540
All	All	0.54	0/14137	0.64	1/19271 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	255	LYS	C-N-CA	5.39	135.17	121.70

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	2876	0	2819	26	0
1	C	2851	0	2797	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	292	0	287	5	0
2	D	292	0	287	7	0
3	E	3445	0	3383	26	0
3	F	3392	0	3342	26	0
4	G	298	0	172	3	0
5	H	311	0	171	0	0
6	A	192	0	288	22	0
6	C	56	0	84	10	0
6	D	8	0	12	1	0
6	E	96	0	144	18	0
6	F	100	0	150	10	0
7	A	45	0	42	2	0
7	C	45	0	42	0	0
8	A	283	0	0	0	0
8	B	8	0	0	0	0
8	C	96	0	0	0	0
8	D	9	0	0	0	0
8	E	174	0	0	0	0
8	F	80	0	0	1	0
8	G	6	0	0	0	0
8	H	13	0	0	0	0
All	All	14968	0	14020	112	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 (112) 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)
3:E:290:GLN:HA	6:E:623:EDO:H12	1.42	0.99
4:G:1:DA:H2"	4:G:2:DA:H5"	1.46	0.95
3:E:146[B]:CYS:SG	6:E:623:EDO:H11	2.18	0.84
1:C:299:LEU:HD23	6:C:403:EDO:H22	1.60	0.83
3:E:193:GLY:H	6:E:602:EDO:H21	1.45	0.80
3:E:106:THR:HB	6:E:607:EDO:H12	1.64	0.80
6:A:433:EDO:H12	3:F:464:GLU:H	1.50	0.74
3:E:517[A]:THR:HG22	3:E:519:THR:HG23	1.75	0.68
6:A:404:EDO:H22	6:A:434:EDO:H12	1.75	0.68
3:E:520:PRO:HD3	6:E:608:EDO:H21	1.76	0.67
3:F:457:GLN:HG3	6:F:609:EDO:H22	1.79	0.64
3:E:520:PRO:CD	6:E:608:EDO:H21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD11	6:A:430:EDO:H21	1.81	0.63
1:A:219:LYS:HE2	6:A:442:EDO:H21	1.79	0.63
3:F:345:MET:HE1	3:F:393:LYS:HB3	1.81	0.62
1:A:98:ARG:O	6:A:434:EDO:H21	1.98	0.62
1:A:274:GLU:HB3	6:A:448:EDO:H12	1.81	0.61
3:F:141:PHE:HB3	6:F:610:EDO:H11	1.83	0.61
3:E:146[B]:CYS:SG	6:E:623:EDO:C1	2.89	0.60
1:A:144:LYS:NZ	6:A:425:EDO:H22	2.16	0.60
3:E:290:GLN:HA	6:E:623:EDO:C1	2.26	0.59
3:E:233:LYS:HE3	6:E:605:EDO:H22	1.84	0.59
2:D:239:LYS:HG3	6:D:302:EDO:H12	1.84	0.58
1:A:165:GLY:HA3	6:A:421:EDO:H11	1.85	0.58
1:A:48:PRO:HB3	6:A:429:EDO:H11	1.86	0.58
1:C:299:LEU:CD2	6:C:403:EDO:H22	2.34	0.56
3:E:148:TYR:OH	6:E:623:EDO:H22	2.06	0.56
1:A:325:GLN:O	6:A:412:EDO:H12	2.05	0.56
1:A:286:THR:HA	6:A:430:EDO:H22	1.87	0.56
3:E:117:ARG:HH11	6:E:609:EDO:H22	1.73	0.54
3:F:197:CYS:HA	6:F:622:EDO:H11	1.88	0.54
3:E:438:GLY:N	3:E:439:GLY:HA2	2.23	0.53
3:F:179:ILE:HG22	3:F:210:ARG:HH22	1.73	0.53
3:F:470[B]:ARG:HB3	3:F:474:THR:OG1	2.09	0.53
1:C:31:THR:HB	6:C:409:EDO:H12	1.91	0.52
1:A:273:LYS:HB2	6:A:438:EDO:H22	1.92	0.52
3:F:427:PRO:HA	6:F:607:EDO:H12	1.92	0.51
6:E:604:EDO:H12	6:E:617:EDO:H21	1.93	0.50
3:F:298:LEU:O	3:F:312:ARG:HB3	2.11	0.50
3:F:345:MET:HE3	3:F:387:CYS:HB2	1.94	0.50
3:F:499:PRO:HB2	6:F:611:EDO:H11	1.93	0.50
3:F:328:VAL:HG23	3:F:329:THR:HG23	1.94	0.50
4:G:1:DA:C2'	4:G:2:DA:H5''	2.29	0.49
2:D:263:ARG:HH21	3:E:522:PRO:HD2	1.77	0.49
6:A:404:EDO:C2	6:A:434:EDO:H12	2.42	0.49
1:C:305:LYS:O	1:C:309:GLU:HG2	2.12	0.49
1:C:212:ILE:HG12	6:C:402:EDO:H12	1.93	0.49
1:A:144:LYS:CE	6:A:425:EDO:H22	2.42	0.49
1:A:26:LYS:HD2	6:A:401:EDO:H21	1.95	0.49
1:C:79:ILE:HG22	1:C:81:PRO:HD3	1.95	0.48
3:E:364:MET:HB3	6:E:612:EDO:H22	1.93	0.48
3:F:504:ARG:HD3	6:F:616:EDO:H12	1.96	0.48
3:F:345:MET:CE	3:F:387:CYS:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HG22	1:A:81:PRO:HD3	1.95	0.48
3:F:317:HIS:HA	3:F:353:PRO:HA	1.96	0.48
1:A:148:MET:HB2	1:A:222:THR:HG21	1.96	0.47
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.95	0.47
2:D:256:SER:HB3	2:D:257:GLY:HA3	1.97	0.47
3:E:218:LYS:HD3	6:E:613:EDO:H11	1.97	0.47
1:C:148:MET:HB2	1:C:222:THR:HG21	1.97	0.47
3:F:482:ILE:HG13	6:F:624:EDO:H11	1.97	0.47
1:C:49:GLN:HE22	6:C:404:EDO:H12	1.79	0.46
3:F:426:THR:HG22	3:F:428:VAL:HG23	1.97	0.46
2:D:243:PHE:HZ	2:D:246:GLU:HB2	1.81	0.46
3:E:438:GLY:H	3:E:439:GLY:HA2	1.80	0.46
2:D:256:SER:HB3	2:D:257:GLY:CA	2.46	0.46
2:D:261:VAL:HG11	2:D:263:ARG:NH1	2.31	0.45
3:E:265:ASN:HA	6:E:620:EDO:H12	1.98	0.45
4:G:1:DA:H2"	4:G:2:DA:C5'	2.33	0.45
1:A:68:GLY:HA3	1:A:332:ASN:O	2.17	0.45
6:A:405:EDO:H22	7:A:449:MTT:H231	1.99	0.45
2:B:243:PHE:HZ	2:B:246:GLU:HB2	1.81	0.45
2:B:256:SER:HA	2:B:257:GLY:HA3	1.72	0.45
3:E:429:PRO:HA	3:E:451:ASN:HB2	1.98	0.45
3:E:307:GLU:HG3	6:E:619:EDO:H21	1.99	0.44
3:F:345:MET:HE3	3:F:395:MET:HG3	1.99	0.44
1:A:48:PRO:HB2	3:F:481:GLU:HG2	2.00	0.44
2:B:258:TRP:HZ2	6:F:624:EDO:H12	1.83	0.44
1:A:277:LYS:HE3	6:A:437:EDO:H12	2.00	0.43
1:C:331:PRO:HA	6:C:407:EDO:H21	1.99	0.43
3:F:121:VAL:HB	3:F:150:PHE:HB2	1.99	0.43
1:C:298:PRO:O	6:C:403:EDO:H11	2.18	0.43
1:C:232:TRP:HB2	1:C:298:PRO:HG2	2.00	0.43
3:E:131:GLN:HB3	6:E:618:EDO:H21	2.00	0.43
3:E:148:TYR:OH	6:E:623:EDO:C2	2.66	0.43
1:A:274:GLU:O	6:A:448:EDO:H21	2.19	0.43
1:C:68:GLY:HA3	1:C:332:ASN:O	2.17	0.43
1:A:200:LYS:O	6:A:447:EDO:H11	2.18	0.43
1:A:243:GLY:HA2	6:A:436:EDO:H12	2.00	0.42
1:A:17:TYR:HD1	6:A:428:EDO:H21	1.84	0.42
3:E:116:GLU:HG2	3:E:116:GLU:H	1.71	0.42
2:D:255:LYS:CB	2:D:256:SER:HA	2.49	0.42
3:F:179:ILE:HG22	3:F:210:ARG:NH2	2.34	0.42
3:F:511:ALA:HB1	6:F:611:EDO:H21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:470[A]:ARG:HB3	3:F:470[A]:ARG:HH11	1.83	0.42
3:E:99:HIS:HA	3:E:100:ILE:HA	1.92	0.42
2:B:253:GLY:HA2	2:B:254:ASP:HA	1.84	0.42
3:F:129:VAL:HB	3:F:238:ILE:HG12	2.02	0.42
1:A:346:ALA:HB2	1:A:364:ALA:HB2	2.01	0.42
1:C:346:ALA:HB2	1:C:364:ALA:HB2	2.02	0.42
1:A:37:VAL:HB	6:A:428:EDO:H22	2.02	0.41
1:A:233[A]:SER:OG	1:A:298:PRO:HD3	2.20	0.41
3:E:121:VAL:HB	3:E:150:PHE:HB2	2.02	0.41
3:E:100:ILE:HA	3:E:422:ALA:HB2	2.01	0.41
1:A:129:TRP:HA	1:A:132:ILE:HD12	2.03	0.41
1:C:332:ASN:H	6:C:407:EDO:H21	1.86	0.41
1:C:321:MET:HG3	6:C:408:EDO:H21	2.03	0.41
7:A:449:MTT:H151	7:A:449:MTT:H262	2.03	0.40
6:F:609:EDO:H12	8:F:716:HOH:O	2.21	0.40
1:C:275:LEU:H	6:C:406:EDO:H11	1.85	0.40
3:F:123:VAL:HB	3:F:148:TYR:HB2	2.03	0.40
2:B:258:TRP:O	3:F:436:LEU:HD21	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	373/370 (101%)	369 (99%)	4 (1%)	0	100	100
1	C	370/370 (100%)	362 (98%)	7 (2%)	1 (0%)	46	41
2	B	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	D	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
3	E	433/424 (102%)	422 (98%)	10 (2%)	1 (0%)	52	50
3	F	425/424 (100%)	415 (98%)	7 (2%)	3 (1%)	26	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1673/1664 (100%)	1632 (98%)	36 (2%)	5 (0%)	46	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	185	ASP
1	C	173	ALA
3	E	100	ILE
3	F	343	LYS
3	F	439	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/292 (100%)	290 (100%)	1 (0%)	94	97
1	C	287/292 (98%)	284 (99%)	3 (1%)	82	85
2	B	28/32 (88%)	27 (96%)	1 (4%)	42	39
2	D	28/32 (88%)	27 (96%)	1 (4%)	42	39
3	E	378/370 (102%)	371 (98%)	7 (2%)	65	68
3	F	373/370 (101%)	364 (98%)	9 (2%)	57	58
All	All	1385/1388 (100%)	1363 (98%)	22 (2%)	72	74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
2	B	234	ARG
1	C	36	THR
1	C	258	PHE
1	C	308	GLU
2	D	234	ARG
3	E	116	GLU

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Mol	Chain	Res	Type
3	E	184	GLN
3	E	240	LYS
3	E	252	ASP
3	E	308	GLU
3	E	423	SER
3	E	468	MET
3	F	181	SER
3	F	184	GLN
3	F	226	ASP
3	F	250	ASN
3	F	423	SER
3	F	468	MET
3	F	470[A]	ARG
3	F	470[B]	ARG
3	F	521	GLU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

115 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	$\# Z > 2$
6	EDO	A	401	-	3,3,3	0.48	0	2,2,2	0.25	0
6	EDO	A	402	-	3,3,3	0.40	0	2,2,2	0.65	0
6	EDO	A	403	-	3,3,3	0.52	0	2,2,2	0.91	0
6	EDO	A	404	-	3,3,3	0.43	0	2,2,2	0.59	0
6	EDO	A	405	-	3,3,3	0.59	0	2,2,2	0.16	0
6	EDO	A	406	-	3,3,3	0.40	0	2,2,2	0.47	0
6	EDO	A	407	-	3,3,3	0.62	0	2,2,2	0.31	0
6	EDO	A	408	-	3,3,3	0.48	0	2,2,2	0.79	0
6	EDO	A	409	-	3,3,3	0.50	0	2,2,2	0.35	0
6	EDO	A	410	-	3,3,3	0.54	0	2,2,2	0.27	0
6	EDO	A	411	-	3,3,3	0.55	0	2,2,2	0.33	0
6	EDO	A	412	-	3,3,3	0.50	0	2,2,2	0.52	0
6	EDO	A	413	-	3,3,3	0.47	0	2,2,2	0.35	0
6	EDO	A	414	-	3,3,3	0.60	0	2,2,2	0.19	0
6	EDO	A	415	-	3,3,3	0.53	0	2,2,2	0.42	0
6	EDO	A	416	-	3,3,3	0.64	0	2,2,2	0.23	0
6	EDO	A	417	-	3,3,3	0.83	0	2,2,2	0.16	0
6	EDO	A	418	-	3,3,3	0.52	0	2,2,2	0.47	0
6	EDO	A	419	-	3,3,3	0.59	0	2,2,2	0.25	0
6	EDO	A	420	-	3,3,3	0.48	0	2,2,2	0.52	0
6	EDO	A	421	-	3,3,3	0.52	0	2,2,2	0.49	0
6	EDO	A	422	-	3,3,3	0.67	0	2,2,2	0.19	0
6	EDO	A	423	-	3,3,3	0.52	0	2,2,2	0.20	0
6	EDO	A	424	-	3,3,3	0.67	0	2,2,2	0.02	0
6	EDO	A	425	-	3,3,3	0.63	0	2,2,2	0.49	0
6	EDO	A	426	-	3,3,3	0.65	0	2,2,2	0.30	0
6	EDO	A	427	-	3,3,3	0.44	0	2,2,2	0.58	0
6	EDO	A	428	-	3,3,3	0.56	0	2,2,2	0.27	0
6	EDO	A	429	-	3,3,3	0.70	0	2,2,2	0.37	0
6	EDO	A	430	-	3,3,3	0.34	0	2,2,2	0.64	0
6	EDO	A	431	-	3,3,3	0.50	0	2,2,2	0.30	0
6	EDO	A	432	-	3,3,3	0.56	0	2,2,2	0.13	0
6	EDO	A	433	-	3,3,3	0.53	0	2,2,2	0.31	0
6	EDO	A	434	-	3,3,3	0.58	0	2,2,2	0.67	0
6	EDO	A	435	-	3,3,3	0.49	0	2,2,2	0.29	0
6	EDO	A	436	-	3,3,3	0.34	0	2,2,2	0.52	0
6	EDO	A	437	-	3,3,3	0.40	0	2,2,2	0.49	0
6	EDO	A	438	-	3,3,3	0.71	0	2,2,2	0.14	0
6	EDO	A	439	-	3,3,3	0.61	0	2,2,2	0.18	0
6	EDO	A	440	-	3,3,3	0.53	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	441	-	3,3,3	0.51	0	2,2,2	0.25	0
6	EDO	A	442	-	3,3,3	0.60	0	2,2,2	0.39	0
6	EDO	A	443	-	3,3,3	0.50	0	2,2,2	0.49	0
6	EDO	A	444	-	3,3,3	0.63	0	2,2,2	0.15	0
6	EDO	A	445	-	3,3,3	0.56	0	2,2,2	0.40	0
6	EDO	A	446	-	3,3,3	0.59	0	2,2,2	0.44	0
6	EDO	A	447	-	3,3,3	0.50	0	2,2,2	0.44	0
6	EDO	A	448	-	3,3,3	0.52	0	2,2,2	0.37	0
7	MTT	A	449	-	48,48,48	0.71	0	71,71,71	1.04	5 (7%)
6	EDO	C	401	-	3,3,3	0.50	0	2,2,2	0.35	0
6	EDO	C	402	-	3,3,3	0.59	0	2,2,2	0.36	0
6	EDO	C	403	-	3,3,3	0.38	0	2,2,2	0.45	0
6	EDO	C	404	-	3,3,3	0.45	0	2,2,2	0.56	0
6	EDO	C	405	-	3,3,3	0.47	0	2,2,2	0.57	0
6	EDO	C	406	-	3,3,3	0.61	0	2,2,2	0.31	0
6	EDO	C	407	-	3,3,3	0.63	0	2,2,2	0.29	0
6	EDO	C	408	-	3,3,3	0.63	0	2,2,2	0.27	0
6	EDO	C	409	-	3,3,3	0.58	0	2,2,2	0.37	0
6	EDO	C	410	-	3,3,3	0.57	0	2,2,2	0.17	0
6	EDO	C	411	-	3,3,3	0.61	0	2,2,2	0.34	0
6	EDO	C	412	-	3,3,3	0.58	0	2,2,2	0.31	0
6	EDO	C	413	-	3,3,3	0.53	0	2,2,2	0.66	0
6	EDO	C	414	-	3,3,3	0.54	0	2,2,2	0.44	0
7	MTT	C	415	-	48,48,48	0.61	0	71,71,71	1.06	3 (4%)
6	EDO	D	301	-	3,3,3	0.53	0	2,2,2	0.39	0
6	EDO	D	302	-	3,3,3	0.55	0	2,2,2	0.35	0
6	EDO	E	601	-	3,3,3	0.63	0	2,2,2	0.38	0
6	EDO	E	602	-	3,3,3	0.53	0	2,2,2	0.48	0
6	EDO	E	603	-	3,3,3	0.56	0	2,2,2	0.30	0
6	EDO	E	604	-	3,3,3	0.47	0	2,2,2	0.40	0
6	EDO	E	605	-	3,3,3	0.43	0	2,2,2	0.57	0
6	EDO	E	606	-	3,3,3	0.51	0	2,2,2	0.49	0
6	EDO	E	607	-	3,3,3	0.56	0	2,2,2	0.30	0
6	EDO	E	608	-	3,3,3	0.56	0	2,2,2	0.52	0
6	EDO	E	609	-	3,3,3	0.52	0	2,2,2	0.38	0
6	EDO	E	610	-	3,3,3	0.44	0	2,2,2	0.48	0
6	EDO	E	611	-	3,3,3	0.64	0	2,2,2	0.21	0
6	EDO	E	612	-	3,3,3	0.58	0	2,2,2	0.27	0
6	EDO	E	613	-	3,3,3	0.46	0	2,2,2	0.51	0
6	EDO	E	614	-	3,3,3	0.55	0	2,2,2	0.45	0
6	EDO	E	615	-	3,3,3	0.65	0	2,2,2	0.26	0
6	EDO	E	616	-	3,3,3	0.47	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	E	617	-	3,3,3	0.58	0	2,2,2	0.27	0
6	EDO	E	618	-	3,3,3	0.44	0	2,2,2	0.27	0
6	EDO	E	619	-	3,3,3	0.55	0	2,2,2	0.36	0
6	EDO	E	620	-	3,3,3	0.44	0	2,2,2	0.60	0
6	EDO	E	621	-	3,3,3	0.54	0	2,2,2	0.58	0
6	EDO	E	622	-	3,3,3	0.48	0	2,2,2	0.42	0
6	EDO	E	623	-	3,3,3	0.64	0	2,2,2	0.02	0
6	EDO	E	624	-	3,3,3	0.61	0	2,2,2	0.29	0
6	EDO	F	601	-	3,3,3	0.55	0	2,2,2	0.41	0
6	EDO	F	602	-	3,3,3	0.61	0	2,2,2	0.48	0
6	EDO	F	603	-	3,3,3	0.55	0	2,2,2	0.34	0
6	EDO	F	604	-	3,3,3	0.53	0	2,2,2	0.40	0
6	EDO	F	605	-	3,3,3	0.62	0	2,2,2	0.16	0
6	EDO	F	606	-	3,3,3	0.54	0	2,2,2	0.39	0
6	EDO	F	607	-	3,3,3	0.46	0	2,2,2	0.70	0
6	EDO	F	608	-	3,3,3	0.56	0	2,2,2	0.49	0
6	EDO	F	609	-	3,3,3	0.62	0	2,2,2	0.27	0
6	EDO	F	610	-	3,3,3	0.65	0	2,2,2	0.48	0
6	EDO	F	611	-	3,3,3	0.61	0	2,2,2	0.32	0
6	EDO	F	612	-	3,3,3	0.48	0	2,2,2	0.52	0
6	EDO	F	613	-	3,3,3	0.57	0	2,2,2	0.24	0
6	EDO	F	614	-	3,3,3	0.56	0	2,2,2	0.17	0
6	EDO	F	615	-	3,3,3	0.55	0	2,2,2	0.35	0
6	EDO	F	616	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	F	617	-	3,3,3	0.50	0	2,2,2	0.37	0
6	EDO	F	618	-	3,3,3	0.55	0	2,2,2	0.29	0
6	EDO	F	619	-	3,3,3	0.54	0	2,2,2	0.29	0
6	EDO	F	620	-	3,3,3	0.54	0	2,2,2	0.38	0
6	EDO	F	621	-	3,3,3	0.57	0	2,2,2	0.29	0
6	EDO	F	622	-	3,3,3	0.68	0	2,2,2	0.17	0
6	EDO	F	623	-	3,3,3	0.54	0	2,2,2	0.37	0
6	EDO	F	624	-	3,3,3	0.45	0	2,2,2	0.73	0
6	EDO	F	625	-	3,3,3	0.54	0	2,2,2	0.43	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	EDO	A	401	-	-	0/1/1/1	0/0/0/0
6	EDO	A	402	-	-	0/1/1/1	0/0/0/0
6	EDO	A	403	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	404	-	-	0/1/1/1	0/0/0/0
6	EDO	A	405	-	-	0/1/1/1	0/0/0/0
6	EDO	A	406	-	-	0/1/1/1	0/0/0/0
6	EDO	A	407	-	-	0/1/1/1	0/0/0/0
6	EDO	A	408	-	-	0/1/1/1	0/0/0/0
6	EDO	A	409	-	-	0/1/1/1	0/0/0/0
6	EDO	A	410	-	-	0/1/1/1	0/0/0/0
6	EDO	A	411	-	-	0/1/1/1	0/0/0/0
6	EDO	A	412	-	-	0/1/1/1	0/0/0/0
6	EDO	A	413	-	-	0/1/1/1	0/0/0/0
6	EDO	A	414	-	-	0/1/1/1	0/0/0/0
6	EDO	A	415	-	-	0/1/1/1	0/0/0/0
6	EDO	A	416	-	-	0/1/1/1	0/0/0/0
6	EDO	A	417	-	-	0/1/1/1	0/0/0/0
6	EDO	A	418	-	-	0/1/1/1	0/0/0/0
6	EDO	A	419	-	-	0/1/1/1	0/0/0/0
6	EDO	A	420	-	-	0/1/1/1	0/0/0/0
6	EDO	A	421	-	-	0/1/1/1	0/0/0/0
6	EDO	A	422	-	-	0/1/1/1	0/0/0/0
6	EDO	A	423	-	-	0/1/1/1	0/0/0/0
6	EDO	A	424	-	-	0/1/1/1	0/0/0/0
6	EDO	A	425	-	-	0/1/1/1	0/0/0/0
6	EDO	A	426	-	-	0/1/1/1	0/0/0/0
6	EDO	A	427	-	-	0/1/1/1	0/0/0/0
6	EDO	A	428	-	-	0/1/1/1	0/0/0/0
6	EDO	A	429	-	-	0/1/1/1	0/0/0/0
6	EDO	A	430	-	-	0/1/1/1	0/0/0/0
6	EDO	A	431	-	-	0/1/1/1	0/0/0/0
6	EDO	A	432	-	-	0/1/1/1	0/0/0/0
6	EDO	A	433	-	-	0/1/1/1	0/0/0/0
6	EDO	A	434	-	-	0/1/1/1	0/0/0/0
6	EDO	A	435	-	-	0/1/1/1	0/0/0/0
6	EDO	A	436	-	-	0/1/1/1	0/0/0/0
6	EDO	A	437	-	-	0/1/1/1	0/0/0/0
6	EDO	A	438	-	-	0/1/1/1	0/0/0/0
6	EDO	A	439	-	-	0/1/1/1	0/0/0/0
6	EDO	A	440	-	-	0/1/1/1	0/0/0/0
6	EDO	A	441	-	-	0/1/1/1	0/0/0/0
6	EDO	A	442	-	-	0/1/1/1	0/0/0/0
6	EDO	A	443	-	-	0/1/1/1	0/0/0/0
6	EDO	A	444	-	-	0/1/1/1	0/0/0/0
6	EDO	A	445	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	446	-	-	0/1/1/1	0/0/0/0
6	EDO	A	447	-	-	0/1/1/1	0/0/0/0
6	EDO	A	448	-	-	0/1/1/1	0/0/0/0
7	MTT	A	449	-	-	0/20/100/100	0/4/4/4
6	EDO	C	401	-	-	0/1/1/1	0/0/0/0
6	EDO	C	402	-	-	0/1/1/1	0/0/0/0
6	EDO	C	403	-	-	0/1/1/1	0/0/0/0
6	EDO	C	404	-	-	0/1/1/1	0/0/0/0
6	EDO	C	405	-	-	0/1/1/1	0/0/0/0
6	EDO	C	406	-	-	0/1/1/1	0/0/0/0
6	EDO	C	407	-	-	0/1/1/1	0/0/0/0
6	EDO	C	408	-	-	0/1/1/1	0/0/0/0
6	EDO	C	409	-	-	0/1/1/1	0/0/0/0
6	EDO	C	410	-	-	0/1/1/1	0/0/0/0
6	EDO	C	411	-	-	0/1/1/1	0/0/0/0
6	EDO	C	412	-	-	0/1/1/1	0/0/0/0
6	EDO	C	413	-	-	0/1/1/1	0/0/0/0
6	EDO	C	414	-	-	0/1/1/1	0/0/0/0
7	MTT	C	415	-	-	0/20/100/100	0/4/4/4
6	EDO	D	301	-	-	0/1/1/1	0/0/0/0
6	EDO	D	302	-	-	0/1/1/1	0/0/0/0
6	EDO	E	601	-	-	0/1/1/1	0/0/0/0
6	EDO	E	602	-	-	0/1/1/1	0/0/0/0
6	EDO	E	603	-	-	0/1/1/1	0/0/0/0
6	EDO	E	604	-	-	0/1/1/1	0/0/0/0
6	EDO	E	605	-	-	0/1/1/1	0/0/0/0
6	EDO	E	606	-	-	0/1/1/1	0/0/0/0
6	EDO	E	607	-	-	0/1/1/1	0/0/0/0
6	EDO	E	608	-	-	0/1/1/1	0/0/0/0
6	EDO	E	609	-	-	0/1/1/1	0/0/0/0
6	EDO	E	610	-	-	0/1/1/1	0/0/0/0
6	EDO	E	611	-	-	0/1/1/1	0/0/0/0
6	EDO	E	612	-	-	0/1/1/1	0/0/0/0
6	EDO	E	613	-	-	0/1/1/1	0/0/0/0
6	EDO	E	614	-	-	0/1/1/1	0/0/0/0
6	EDO	E	615	-	-	0/1/1/1	0/0/0/0
6	EDO	E	616	-	-	0/1/1/1	0/0/0/0
6	EDO	E	617	-	-	0/1/1/1	0/0/0/0
6	EDO	E	618	-	-	0/1/1/1	0/0/0/0
6	EDO	E	619	-	-	0/1/1/1	0/0/0/0
6	EDO	E	620	-	-	0/1/1/1	0/0/0/0
6	EDO	E	621	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	622	-	-	0/1/1/1	0/0/0/0
6	EDO	E	623	-	-	0/1/1/1	0/0/0/0
6	EDO	E	624	-	-	0/1/1/1	0/0/0/0
6	EDO	F	601	-	-	0/1/1/1	0/0/0/0
6	EDO	F	602	-	-	0/1/1/1	0/0/0/0
6	EDO	F	603	-	-	0/1/1/1	0/0/0/0
6	EDO	F	604	-	-	0/1/1/1	0/0/0/0
6	EDO	F	605	-	-	0/1/1/1	0/0/0/0
6	EDO	F	606	-	-	0/1/1/1	0/0/0/0
6	EDO	F	607	-	-	0/1/1/1	0/0/0/0
6	EDO	F	608	-	-	0/1/1/1	0/0/0/0
6	EDO	F	609	-	-	0/1/1/1	0/0/0/0
6	EDO	F	610	-	-	0/1/1/1	0/0/0/0
6	EDO	F	611	-	-	0/1/1/1	0/0/0/0
6	EDO	F	612	-	-	0/1/1/1	0/0/0/0
6	EDO	F	613	-	-	0/1/1/1	0/0/0/0
6	EDO	F	614	-	-	0/1/1/1	0/0/0/0
6	EDO	F	615	-	-	0/1/1/1	0/0/0/0
6	EDO	F	616	-	-	0/1/1/1	0/0/0/0
6	EDO	F	617	-	-	0/1/1/1	0/0/0/0
6	EDO	F	618	-	-	0/1/1/1	0/0/0/0
6	EDO	F	619	-	-	0/1/1/1	0/0/0/0
6	EDO	F	620	-	-	0/1/1/1	0/0/0/0
6	EDO	F	621	-	-	0/1/1/1	0/0/0/0
6	EDO	F	622	-	-	0/1/1/1	0/0/0/0
6	EDO	F	623	-	-	0/1/1/1	0/0/0/0
6	EDO	F	624	-	-	0/1/1/1	0/0/0/0
6	EDO	F	625	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	415	MTT	C12-C13-C14	-2.51	106.16	110.79
7	A	449	MTT	C26-C25-C24	-2.51	105.88	113.25
7	C	415	MTT	C26-C25-C24	-2.34	106.37	113.25
7	A	449	MTT	C12-C13-C14	-2.14	106.84	110.79
7	C	415	MTT	C36-C35-C34	-2.10	107.08	113.25
7	A	449	MTT	C46-C45-C44	-2.09	107.11	113.25
7	A	449	MTT	O14-C14-C13	-2.08	105.67	110.36
7	A	449	MTT	C36-C35-C34	-2.02	107.32	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

46 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	EDO	1	0
6	A	404	EDO	2	0
6	A	405	EDO	1	0
6	A	412	EDO	1	0
6	A	421	EDO	1	0
6	A	425	EDO	2	0
6	A	428	EDO	2	0
6	A	429	EDO	1	0
6	A	430	EDO	2	0
6	A	433	EDO	1	0
6	A	434	EDO	3	0
6	A	436	EDO	1	0
6	A	437	EDO	1	0
6	A	438	EDO	1	0
6	A	442	EDO	1	0
6	A	447	EDO	1	0
6	A	448	EDO	2	0
7	A	449	MTT	2	0
6	C	402	EDO	1	0
6	C	403	EDO	3	0
6	C	404	EDO	1	0
6	C	406	EDO	1	0
6	C	407	EDO	2	0
6	C	408	EDO	1	0
6	C	409	EDO	1	0
6	D	302	EDO	1	0
6	E	602	EDO	1	0
6	E	604	EDO	1	0
6	E	605	EDO	1	0
6	E	607	EDO	1	0
6	E	608	EDO	2	0
6	E	609	EDO	1	0
6	E	612	EDO	1	0
6	E	613	EDO	1	0
6	E	617	EDO	1	0
6	E	618	EDO	1	0
6	E	619	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	620	EDO	1	0
6	E	623	EDO	6	0
6	F	607	EDO	1	0
6	F	609	EDO	2	0
6	F	610	EDO	1	0
6	F	611	EDO	2	0
6	F	616	EDO	1	0
6	F	622	EDO	1	0
6	F	624	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th 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	370/370 (100%)	-0.20	0 100 100	19, 30, 51, 82	0
1	C	370/370 (100%)	0.23	19 (5%) 32 41	36, 59, 99, 123	0
2	B	38/38 (100%)	0.98	7 (18%) 2 3	36, 58, 119, 122	0
2	D	38/38 (100%)	0.93	6 (15%) 3 4	38, 56, 114, 116	0
3	E	424/424 (100%)	0.08	20 (4%) 35 45	25, 44, 83, 122	0
3	F	422/424 (99%)	0.55	48 (11%) 7 10	28, 60, 115, 161	0
4	G	15/15 (100%)	-0.14	0 100 100	47, 60, 72, 75	0
5	H	15/15 (100%)	-0.42	0 100 100	38, 57, 70, 73	0
All	All	1692/1694 (99%)	0.20	100 (5%) 26 34	19, 49, 98, 161	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	311	VAL	8.5
3	F	181	SER	8.4
2	D	252	ASP	8.2
3	F	247	SER	8.1
2	B	253	GLY	7.8
1	C	172	ALA	7.0
2	B	252	ASP	7.0
3	E	100	ILE	6.7
3	F	134	TYR	6.4
2	D	254	ASP	6.3
2	D	256	SER	6.3
2	B	254	ASP	6.2
3	F	251	ALA	6.0
1	C	174	GLY	6.0
3	E	438	GLY	5.9
3	E	439	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
3	E	99	HIS	5.5
2	D	255	LYS	5.5
1	C	173	ALA	5.5
2	D	253	GLY	5.3
3	F	439	GLY	5.1
3	E	271	THR	4.9
3	F	135	GLY	4.9
3	F	184	GLN	4.8
3	F	391	PRO	4.6
3	F	249	LYS	4.6
3	E	243	LYS	4.4
1	C	84	ALA	4.4
3	F	248	LEU	4.4
3	F	244	LYS	4.3
3	F	441	ASP	4.3
3	F	246	GLN	4.2
3	F	209	LYS	4.2
3	F	252	ASP	4.2
3	F	243	LYS	4.2
2	D	251	LYS	4.1
3	F	241	PRO	4.1
3	F	183	ASP	4.0
1	C	239	ALA	4.0
3	F	387	CYS	3.8
1	C	313	LYS	3.8
3	F	245	LYS	3.8
1	C	92	PHE	3.8
3	E	441	ASP	3.7
1	C	171	TYR	3.7
3	F	250	ASN	3.6
3	F	136	ASN	3.5
1	C	175	LYS	3.5
2	B	250	SER	3.4
1	C	178	ILE	3.4
3	F	101	GLU	3.2
3	F	240	LYS	3.2
3	F	302	ASN	3.1
1	C	87	ASP	3.1
1	C	90	TYR	3.1
3	E	442	VAL	3.1
3	F	388	PRO	3.0
3	F	309	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	385	THR	2.9
3	F	180	GLY	2.9
3	F	163	GLN	2.9
2	B	251	LYS	2.8
1	C	226	ILE	2.8
3	F	310	GLN	2.8
1	C	169	PHE	2.8
3	F	404	ILE	2.7
1	C	252	GLY	2.7
2	B	256	SER	2.7
3	F	242	SER	2.6
3	E	263	LEU	2.6
3	E	391	PRO	2.6
3	F	103	LYS	2.6
3	E	422	ALA	2.6
2	B	255	LYS	2.6
3	F	211	LYS	2.6
3	F	315	TYR	2.5
3	F	207	SER	2.5
3	E	249	LYS	2.5
3	E	269	SER	2.5
3	F	390	GLU	2.5
1	C	179	LYS	2.5
1	C	170	LYS	2.5
3	F	384	ALA	2.4
3	F	395	MET	2.4
3	F	212	HIS	2.4
3	E	242	SER	2.4
3	F	182	SER	2.4
3	F	386	PRO	2.3
3	E	404	ILE	2.3
3	E	101	GLU	2.3
3	F	343	LYS	2.2
3	E	401[A]	CYS	2.2
3	E	268	ARG	2.2
1	C	156	PHE	2.1
1	C	155	TYR	2.1
3	E	389	LYS	2.1
3	F	389	LYS	2.1
3	F	422	ALA	2.0
3	E	248	LEU	2.0
3	F	312	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	EDO	E	608	4/4	0.88	0.39	24.14	55,56,56,60	0
6	EDO	A	442	4/4	0.87	0.41	21.78	66,66,66,67	0
6	EDO	C	408	4/4	0.66	0.33	18.25	77,77,78,79	0
6	EDO	C	412	4/4	0.82	0.27	17.77	75,76,77,77	0
6	EDO	A	446	4/4	0.73	0.45	15.94	66,67,68,68	0
6	EDO	F	614	4/4	0.67	0.51	15.34	76,77,78,78	0
6	EDO	A	426	4/4	0.87	0.29	14.27	45,51,53,54	0
6	EDO	A	430	4/4	0.94	0.42	14.26	58,58,61,62	0
6	EDO	A	434	4/4	0.86	0.42	12.58	42,47,52,54	0
6	EDO	A	443	4/4	0.93	0.33	12.20	60,61,62,64	0
6	EDO	A	428	4/4	0.87	0.27	12.12	62,63,64,64	0
6	EDO	A	421	4/4	0.94	0.25	11.83	57,61,65,69	0
6	EDO	A	437	4/4	0.77	0.29	10.76	82,82,82,82	0
6	EDO	E	617	4/4	0.63	0.34	10.24	89,89,90,90	0
6	EDO	C	403	4/4	0.95	0.36	10.24	45,47,48,51	0
6	EDO	E	616	4/4	0.89	0.29	9.99	69,70,72,73	0
6	EDO	E	623	4/4	0.82	0.32	9.94	47,52,59,63	0
6	EDO	A	411	4/4	0.91	0.39	9.27	65,67,68,69	0
6	EDO	E	612	4/4	0.76	0.32	9.23	51,55,58,59	0
6	EDO	A	412	4/4	0.93	0.32	9.03	50,50,52,54	0
6	EDO	A	416	4/4	0.65	0.30	8.74	65,67,70,73	0
6	EDO	F	622	4/4	0.80	0.43	8.68	64,66,66,67	0
6	EDO	A	424	4/4	0.71	0.29	8.45	59,63,66,66	0
6	EDO	F	617	4/4	0.85	0.38	8.41	76,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	EDO	A	432	4/4	0.87	0.41	8.34	55,57,58,60	0
6	EDO	A	438	4/4	0.87	0.27	8.34	38,41,43,45	0
6	EDO	F	618	4/4	0.86	0.32	8.02	52,53,57,59	0
6	EDO	A	425	4/4	0.90	0.26	7.54	43,43,46,49	0
6	EDO	C	405	4/4	0.89	0.42	7.20	75,76,77,78	0
6	EDO	A	441	4/4	0.85	0.22	7.17	67,68,68,69	0
6	EDO	E	622	4/4	0.89	0.29	7.07	65,65,66,68	0
6	EDO	F	611	4/4	0.87	0.33	6.90	57,57,57,58	0
6	EDO	A	407	4/4	0.76	0.23	6.88	63,64,65,65	0
6	EDO	A	448	4/4	0.86	0.23	6.34	42,48,51,57	0
6	EDO	C	409	4/4	0.68	0.30	5.92	68,69,69,69	0
6	EDO	E	621	4/4	0.93	0.17	5.70	63,63,64,64	0
6	EDO	C	401	4/4	0.90	0.39	5.46	80,80,81,81	0
6	EDO	A	436	4/4	0.75	0.23	5.29	53,56,60,61	0
6	EDO	A	420	4/4	0.80	0.27	5.10	72,73,76,78	0
6	EDO	A	431	4/4	0.89	0.30	4.80	58,59,60,60	0
6	EDO	F	605	4/4	0.93	0.26	4.39	64,65,66,66	0
6	EDO	A	433	4/4	0.86	0.33	4.22	54,58,58,59	0
6	EDO	F	609	4/4	0.90	0.22	4.12	51,56,57,59	0
6	EDO	A	414	4/4	0.88	0.30	4.12	52,56,61,63	0
6	EDO	E	610	4/4	0.86	0.21	4.07	72,72,73,73	0
6	EDO	E	619	4/4	0.85	0.43	3.94	73,74,74,74	0
6	EDO	C	404	4/4	0.86	0.25	3.71	59,63,66,70	0
6	EDO	E	624	4/4	0.83	0.32	3.29	68,69,69,70	0
6	EDO	A	401	4/4	0.96	0.14	3.22	50,51,51,54	0
6	EDO	E	605	4/4	0.94	0.19	2.97	50,50,52,54	0
6	EDO	C	407	4/4	0.75	0.20	2.88	70,72,73,74	0
6	EDO	F	607	4/4	0.93	0.22	2.72	70,70,71,71	0
6	EDO	F	623	4/4	0.90	0.21	2.65	71,71,71,71	0
6	EDO	F	613	4/4	0.83	0.38	2.61	67,70,72,74	0
6	EDO	F	610	4/4	0.87	0.20	2.51	56,58,59,59	0
6	EDO	A	403	4/4	0.92	0.19	2.51	38,41,41,45	0
6	EDO	A	408	4/4	0.90	0.17	2.30	43,43,47,47	0
6	EDO	A	429	4/4	0.83	0.25	2.28	37,45,47,52	0
6	EDO	F	624	4/4	0.83	0.25	2.03	47,51,54,56	0
6	EDO	D	301	4/4	0.80	0.24	1.83	84,85,86,86	0
6	EDO	E	618	4/4	0.93	0.25	1.80	46,51,52,55	0
6	EDO	F	616	4/4	0.93	0.19	1.56	73,73,73,73	0
6	EDO	F	604	4/4	0.86	0.18	1.51	73,74,75,76	0
6	EDO	E	614	4/4	0.94	0.15	1.30	60,61,61,62	0
6	EDO	F	608	4/4	0.84	0.19	1.28	61,64,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	EDO	E	602	4/4	0.92	0.15	1.20	55,57,58,59	0
6	EDO	E	620	4/4	0.92	0.22	1.05	50,55,58,62	0
6	EDO	A	415	4/4	0.96	0.12	0.59	43,45,48,49	0
6	EDO	E	604	4/4	0.91	0.12	0.20	64,64,65,66	0
6	EDO	E	603	4/4	0.86	0.13	0.08	63,63,64,65	0
7	MTT	C	415	45/45	0.96	0.15	-0.12	33,36,42,45	0
6	EDO	A	410	4/4	0.91	0.14	-0.16	46,51,54,57	0
6	EDO	A	406	4/4	0.90	0.14	-0.29	56,58,61,63	0
7	MTT	A	449	45/45	0.96	0.14	-0.31	18,24,35,42	0
6	EDO	E	601	4/4	0.95	0.09	-0.52	34,37,37,38	0
6	EDO	F	602	4/4	0.97	0.09	-0.65	29,30,31,31	0
6	EDO	A	404	4/4	0.98	0.09	-0.71	35,36,37,40	0
6	EDO	F	619	4/4	0.81	0.32	-	79,80,81,81	0
6	EDO	C	411	4/4	0.77	0.53	-	76,76,77,77	0
6	EDO	E	615	4/4	0.78	0.29	-	69,71,71,71	0
6	EDO	A	423	4/4	0.76	0.30	-	73,74,75,77	0
6	EDO	A	427	4/4	0.86	0.30	-	75,75,77,77	0
6	EDO	E	606	4/4	0.92	0.14	-	64,65,66,68	0
6	EDO	F	603	4/4	0.88	0.13	-	72,73,74,74	0
6	EDO	F	615	4/4	0.87	0.42	-	65,65,65,67	0
6	EDO	C	413	4/4	0.92	0.21	-	56,60,63,64	0
6	EDO	A	444	4/4	0.76	0.47	-	57,62,65,68	0
6	EDO	A	409	4/4	0.88	0.26	-	63,65,66,67	0
6	EDO	A	417	4/4	0.83	0.25	-	50,51,52,53	0
6	EDO	A	445	4/4	0.72	0.41	-	71,72,72,73	0
6	EDO	E	613	4/4	0.79	0.16	-	59,60,63,66	0
6	EDO	C	414	4/4	0.75	0.60	-	79,80,81,82	0
6	EDO	C	406	4/4	0.75	0.35	-	69,69,69,69	0
6	EDO	E	609	4/4	0.60	0.41	-	79,81,83,84	0
6	EDO	F	601	4/4	0.94	0.21	-	67,67,68,68	0
6	EDO	F	612	4/4	0.88	0.16	-	64,64,65,65	0
6	EDO	D	302	4/4	0.84	0.42	-	79,80,81,81	0
6	EDO	F	620	4/4	0.89	0.31	-	68,69,71,72	0
6	EDO	F	621	4/4	0.65	0.39	-	83,84,84,84	0
6	EDO	C	410	4/4	0.82	0.39	-	64,67,68,69	0
6	EDO	A	440	4/4	0.86	0.38	-	77,77,78,79	0
6	EDO	A	413	4/4	0.78	0.26	-	79,80,80,81	0
6	EDO	A	447	4/4	0.77	0.45	-	63,65,68,71	0
6	EDO	E	611	4/4	0.75	0.45	-	65,67,68,68	0
6	EDO	A	422	4/4	0.74	0.16	-	68,70,73,75	0
6	EDO	A	419	4/4	0.90	0.28	-	46,53,58,62	0
6	EDO	C	402	4/4	0.85	0.44	-	62,63,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	EDO	F	625	4/4	0.86	0.17	-	78,78,78,79	0
6	EDO	A	435	4/4	0.87	0.20	-	40,45,46,47	0
6	EDO	A	439	4/4	0.74	0.39	-	68,69,69,70	0
6	EDO	F	606	4/4	0.93	0.31	-	58,59,60,62	0
6	EDO	E	607	4/4	0.78	0.25	-	66,67,67,68	0
6	EDO	A	405	4/4	0.97	0.11	-	45,48,49,50	0
6	EDO	A	418	4/4	0.72	0.47	-	73,73,73,74	0
6	EDO	A	402	4/4	0.98	0.19	-	47,48,49,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.