



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:29 AM UTC

PDB ID : 4GZ0 / pdb_00004gz0
Title : Mus Musculus Tdp2-DNA Substrate Analog (5'-6-aminohexanol) Complex
Authors : Schellenberg, M.J.; Williams, R.S.
Deposited on : 2012-09-05
Resolution : 2.11 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

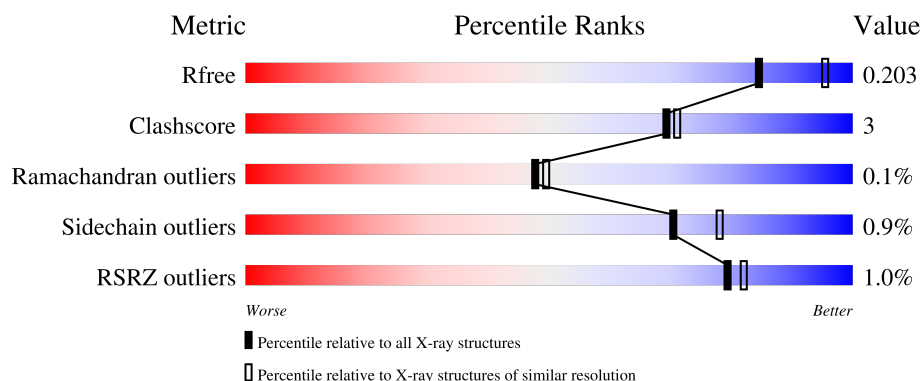
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	256	2% 90% 7%
1	B	256	2% 90% 7%
1	E	256	88% 9%
1	G	256	2% 89% 8%
1	I	256	2% 89% 9%

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Mol	Chain	Length	Quality of chain
1	K	256	% 90% 7% ••
2	C	9	100%
2	D	9	89% 11%
2	F	9	78% 22%
2	H	9	89% 11%
2	J	9	56% 44%
2	L	9	78% 22%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14788 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 Tyrosyl-DNA phosphodiesterase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	5	0
			2005	1278	345	367	15			
1	B	250	Total	C	N	O	S	0	9	0
			2033	1299	348	370	16			
1	E	250	Total	C	N	O	S	0	5	0
			2011	1281	347	368	15			
1	K	249	Total	C	N	O	S	0	5	0
			2006	1279	349	362	16			
1	G	249	Total	C	N	O	S	0	5	0
			1999	1276	343	365	15			
1	I	250	Total	C	N	O	S	0	3	0
			2002	1276	348	363	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	expression tag	UNP Q9JJX7
A	116	ASN	-	expression tag	UNP Q9JJX7
A	117	GLY	-	expression tag	UNP Q9JJX7
B	115	SER	-	expression tag	UNP Q9JJX7
B	116	ASN	-	expression tag	UNP Q9JJX7
B	117	GLY	-	expression tag	UNP Q9JJX7
E	115	SER	-	expression tag	UNP Q9JJX7
E	116	ASN	-	expression tag	UNP Q9JJX7
E	117	GLY	-	expression tag	UNP Q9JJX7
K	115	SER	-	expression tag	UNP Q9JJX7
K	116	ASN	-	expression tag	UNP Q9JJX7
K	117	GLY	-	expression tag	UNP Q9JJX7
G	115	SER	-	expression tag	UNP Q9JJX7
G	116	ASN	-	expression tag	UNP Q9JJX7
G	117	GLY	-	expression tag	UNP Q9JJX7
I	115	SER	-	expression tag	UNP Q9JJX7
I	116	ASN	-	expression tag	UNP Q9JJX7

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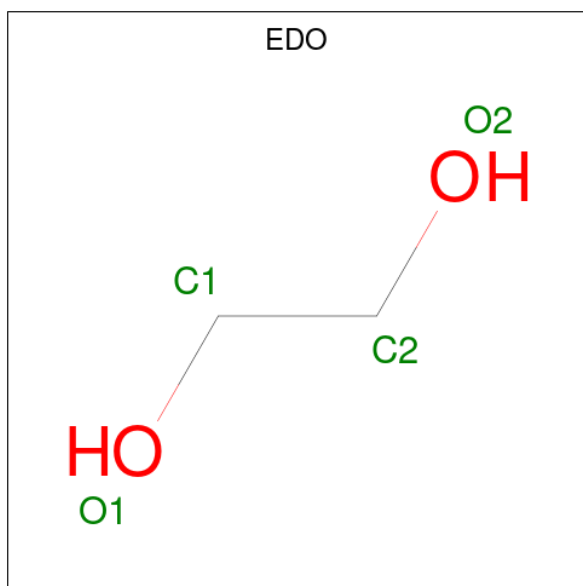
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Chain	Residue	Modelled	Actual	Comment	Reference
I	117	GLY	-	expression tag	UNP Q9JJX7

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			
2	D	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			
2	F	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			
2	L	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			
2	H	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			
2	J	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 8	C 4	O 4	0	1
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

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

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

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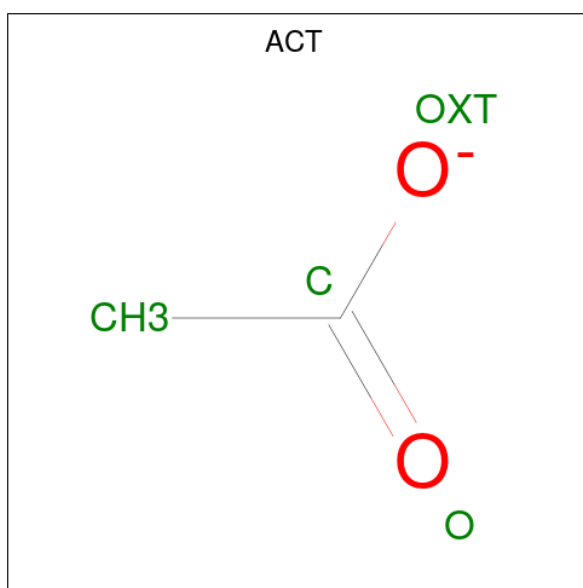
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 8	C 4	O 4	0	1
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



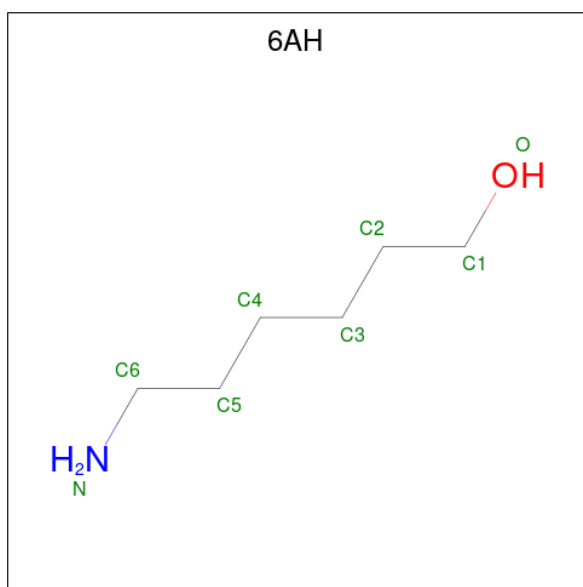
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is 6-aminohexan-1-ol (CCD ID: 6AH) (formula: C₆H₁₅NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			8	6	1	1		
5	D	1	Total	C	N	O	0	0
			8	6	1	1		
5	F	1	Total	C	N	O	0	0
			8	6	1	1		
5	L	1	Total	C	N	O	0	0
			8	6	1	1		
5	H	1	Total	C	O		0	0
			5	4	1			
5	J	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total	O	0	0
			194	194		
6	B	155	Total	O	0	0
			155	155		
6	C	18	Total	O	0	0
			18	18		
6	D	22	Total	O	0	0
			22	22		
6	E	195	Total	O	0	0
			195	195		
6	F	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	126	Total 126	O 126	0	0
6	L	18	Total 18	O 18	0	0
6	G	123	Total 124	O 124	0	1
6	H	21	Total 21	O 21	0	0
6	I	131	Total 131	O 131	0	0
6	J	14	Total 14	O 14	0	0

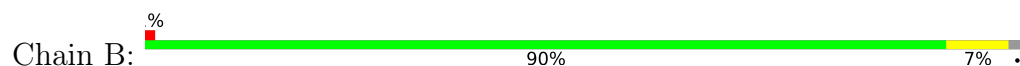
3 Residue-property plots [i](#)

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: Tyrosyl-DNA phosphodiesterase 2



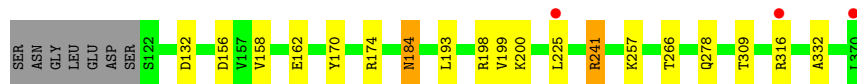
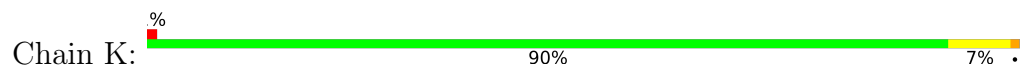
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



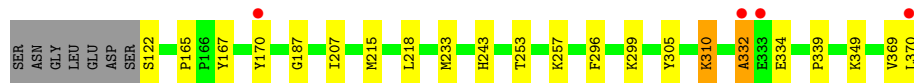
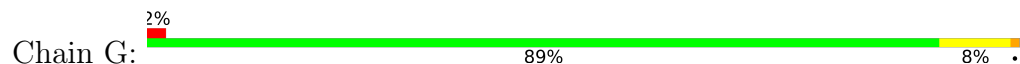
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



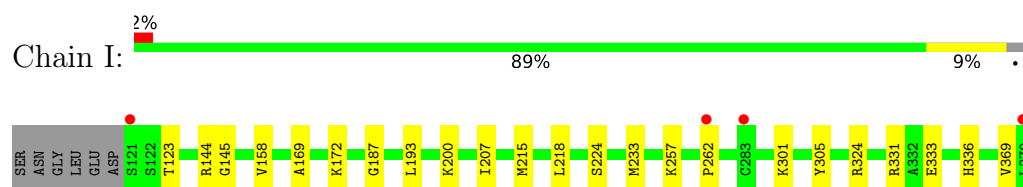
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2

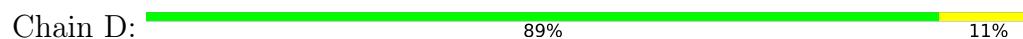


- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')

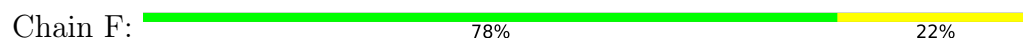


There are no outlier residues recorded for this chain.

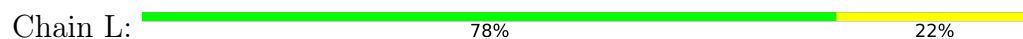
- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')



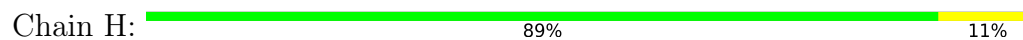
- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')



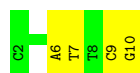
- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(P*CP*CP*GP*AP*AP*TP*TP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.90Å 121.10Å 167.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.24 – 2.11 42.24 – 2.11	Depositor EDS
% Data completeness (in resolution range)	95.5 (42.24-2.11) 95.4 (42.24-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.7.3_928, REFMAC	Depositor
R, R_{free}	0.160 , 0.193 (Not available) , 0.203	Depositor DCC
R_{free} test set	6590 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14788	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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.*

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: 6AH, EDO, ACT

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	0.39	0/2066	0.72	0/2796
1	B	0.36	0/2105	0.72	1/2847 (0.0%)
1	E	0.40	0/2071	0.70	0/2802
1	G	0.36	0/2059	0.75	2/2785 (0.1%)
1	I	0.36	0/2057	0.73	0/2783
1	K	0.33	0/2066	0.72	0/2794
2	C	0.13	0/204	0.58	0/312
2	D	0.14	0/204	0.63	0/312
2	F	0.14	0/204	0.60	0/312
2	H	0.16	0/204	0.64	0/312
2	J	0.17	0/204	0.66	0/312
2	L	0.17	0/204	0.71	0/312
All	All	0.35	0/13648	0.71	3/18679 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	332	ALA	N-CA-C	7.09	125.90	110.80
1	B	165	PRO	N-CA-C	5.26	117.12	110.70
1	G	165	PRO	N-CA-C	5.13	116.96	110.70

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	2005	0	2005	13	0
1	B	2033	0	2052	14	0
1	E	2011	0	2013	17	0
1	G	1999	0	2008	13	0
1	I	2002	0	2004	15	0
1	K	2006	0	2018	14	0
2	C	183	0	102	0	0
2	D	183	0	102	1	0
2	F	183	0	102	2	0
2	H	183	0	102	1	0
2	J	183	0	102	2	0
2	L	183	0	102	1	0
3	A	92	0	138	7	0
3	B	88	0	132	6	0
3	D	12	0	18	2	0
3	E	80	0	120	8	0
3	F	4	0	6	1	0
3	G	44	0	66	2	0
3	H	12	0	18	0	0
3	I	68	0	102	6	0
3	J	4	0	6	0	0
3	K	56	0	84	4	0
4	A	20	0	15	1	0
4	B	12	0	9	1	0
4	E	16	0	12	0	0
4	G	12	0	9	1	0
4	I	16	0	12	1	0
4	K	12	0	9	0	0
5	C	8	0	14	0	0
5	D	8	0	14	0	0
5	F	8	0	14	1	0
5	H	5	0	6	0	0
5	J	8	0	14	0	0
5	L	8	0	14	0	0
6	A	194	0	0	0	0
6	B	155	0	0	2	0
6	C	18	0	0	0	0
6	D	22	0	0	0	0
6	E	195	0	0	0	0
6	F	23	0	0	0	0
6	G	124	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	21	0	0	0	0
6	I	131	0	0	0	0
6	J	14	0	0	0	0
6	K	126	0	0	2	0
6	L	18	0	0	0	0
All	All	14788	0	13544	94	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 3.

All (94) 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:B:151:ALA:HB2	3:B:419:EDO:H11	1.67	0.76
1:B:218:LEU:HD11	1:B:233:MET:HE3	1.72	0.70
1:E:218:LEU:HD11	1:E:233:MET:HE3	1.73	0.69
1:A:218:LEU:HD11	1:A:233:MET:HE3	1.77	0.66
1:G:187:GLY:HA3	1:G:215:MET:HE1	1.78	0.66
1:G:369:VAL:HG12	1:G:370:LEU:HG	1.77	0.65
1:B:304[B]:GLN:NE2	6:B:642:HOH:O	2.27	0.64
1:B:205[B]:GLU:OE2	6:B:577:HOH:O	2.15	0.63
2:L:9:DC:H2'	2:L:10:DG:C8	2.34	0.63
1:E:149[B]:CYS:HG	3:E:414:EDO:HO1	1.47	0.61
1:I:187:GLY:HA3	1:I:215:MET:HE1	1.82	0.61
1:K:241:ARG:HH21	3:K:414:EDO:H21	1.66	0.61
1:I:207:ILE:HD11	1:I:257:LYS:HE3	1.82	0.60
1:A:335:GLY:H	3:A:401:EDO:H12	1.67	0.59
1:I:169:ALA:HB2	3:I:405:EDO:H11	1.87	0.57
1:K:316[B]:ARG:NH1	6:K:583:HOH:O	2.38	0.56
1:G:218:LEU:HD11	1:G:233:MET:HE3	1.87	0.56
3:D:103:EDO:H21	2:H:5:DA:H62	1.71	0.54
1:I:172:LYS:HB3	3:I:415:EDO:H21	1.88	0.54
1:G:243:HIS:HD2	6:G:570:HOH:O	1.91	0.54
1:A:315:LEU:HD12	3:A:412:EDO:H11	1.90	0.54
1:G:207:ILE:HD13	1:G:257:LYS:HE2	1.90	0.54
1:I:262:PRO:O	1:I:331:ARG:NH2	2.42	0.52
2:J:9:DC:H2'	2:J:10:DG:C8	2.45	0.51
1:K:199:VAL:HG22	1:K:225:LEU:HD13	1.93	0.51
1:B:217:ASN:HD22	3:B:417:EDO:H11	1.76	0.50
1:E:199:VAL:HG22	1:E:225:LEU:HD13	1.93	0.50
1:G:122:SER:N	6:G:590:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:TYR:HB2	3:I:404:EDO:H21	1.93	0.50
2:F:5:DA:N7	3:F:102:EDO:O1	2.43	0.50
1:I:333:GLU:HG3	1:I:336[A]:HIS:CG	2.47	0.50
1:A:210:PRO:HD2	3:A:405:EDO:H12	1.94	0.50
1:G:167:TYR:HA	1:G:170:TYR:CD2	2.47	0.48
1:E:304:GLN:HE21	3:E:415:EDO:H11	1.78	0.48
1:E:266:THR:HG23	1:E:332:ALA:HB2	1.95	0.48
1:I:336[B]:HIS:ND1	1:I:369:VAL:O	2.44	0.48
1:E:305:TYR:O	3:E:406:EDO:H12	2.15	0.47
1:I:144:ARG:HH21	3:I:412:EDO:H11	1.80	0.47
1:E:131:ILE:HD12	1:E:167:TYR:CZ	2.50	0.47
1:E:324:ARG:HB3	3:E:415:EDO:H21	1.96	0.46
1:I:145:GLY:HA2	4:I:418:ACT:H2	1.98	0.46
1:E:313:ASN:ND2	3:E:420:EDO:H11	2.31	0.46
1:I:324:ARG:HB3	3:I:416:EDO:H12	1.98	0.45
1:E:158:VAL:HB	1:E:193:LEU:HB2	1.98	0.45
1:B:304[B]:GLN:HG3	1:B:305:TYR:CD2	2.52	0.45
1:B:358:ASP:HB2	3:B:401:EDO:H21	1.98	0.45
1:I:200:LYS:HE2	1:I:224:SER:HB3	1.99	0.45
1:K:170:TYR:CZ	1:K:174:ARG:HD2	2.52	0.45
1:K:257:LYS:HA	1:K:257:LYS:HD3	1.80	0.45
1:K:309:THR:HA	3:K:401:EDO:H12	1.99	0.45
2:J:6:DA:H1'	2:J:7:DT:H5''	1.99	0.45
1:I:158:VAL:HB	1:I:193:LEU:HB2	1.99	0.44
1:A:280:VAL:HG12	1:A:285:GLY:HA2	1.98	0.44
1:A:184:ASN:HA	3:A:421:EDO:H21	1.99	0.44
1:E:347:LEU:H	3:E:414:EDO:H22	1.82	0.44
1:B:180:ILE:HG12	1:B:193:LEU:HG	2.00	0.44
1:G:349:LYS:NZ	4:G:414:ACT:O	2.43	0.44
1:A:334:GLU:HA	3:A:401:EDO:H12	2.00	0.44
1:E:144:ARG:HG2	1:E:170:TYR:OH	2.18	0.44
1:K:170:TYR:CE1	1:K:174:ARG:HD2	2.53	0.44
1:G:310:LYS:HD3	1:G:310:LYS:HA	1.69	0.43
1:B:296:PHE:CE1	1:B:339:PRO:HD2	2.53	0.43
1:K:170:TYR:HB2	3:K:407:EDO:H12	2.00	0.43
1:K:184:ASN:ND2	6:K:612:HOH:O	2.50	0.43
1:E:210:PRO:HD2	3:E:404:EDO:H12	2.01	0.43
1:K:158:VAL:HB	1:K:193:LEU:HB2	2.01	0.43
1:E:324:ARG:CB	3:E:415:EDO:H21	2.48	0.42
1:B:179:THR:HB	4:B:423:ACT:H1	2.00	0.42
1:A:158:VAL:HB	1:A:193:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:LEU:HD11	1:I:233:MET:HE3	2.01	0.42
1:K:266:THR:HG23	1:K:332:ALA:HB2	2.01	0.42
1:K:156:ASP:OD1	1:K:198:ARG:NE	2.51	0.42
1:G:299:LYS:HD2	3:G:404:EDO:H21	2.01	0.42
1:A:266:THR:HG23	1:A:332:ALA:HB2	2.01	0.41
1:G:253:THR:O	1:G:257:LYS:HG2	2.21	0.41
1:B:144:ARG:HG2	1:B:170:TYR:OH	2.19	0.41
1:K:132:ASP:HA	1:K:162:GLU:OE1	2.20	0.41
1:I:324:ARG:CB	3:I:416:EDO:H12	2.50	0.41
1:K:278[B]:GLN:CD	1:K:278[B]:GLN:H	2.28	0.41
2:F:2:DC:H2'	5:F:101:6AH:H5	2.01	0.41
1:B:166:PRO:HB3	3:B:416:EDO:H11	2.02	0.41
2:D:5:DA:H62	3:D:104:EDO:H11	1.85	0.41
1:G:296:PHE:CE2	1:G:339:PRO:HD2	2.56	0.41
1:B:347:LEU:H	3:B:403:EDO:H21	1.85	0.41
1:A:296:PHE:CE1	1:A:339:PRO:HD2	2.56	0.41
3:K:405:EDO:H21	3:K:408:EDO:H22	2.03	0.41
1:A:305:TYR:HB2	3:A:409:EDO:H21	2.03	0.41
1:E:202:LYS:HB3	1:E:202:LYS:HE3	1.86	0.41
1:E:207:ILE:HB	1:E:218:LEU:HB3	2.03	0.41
1:E:233:MET:HE1	1:E:254:VAL:HG13	2.02	0.41
1:G:305:TYR:HB2	3:G:405:EDO:H12	2.02	0.41
1:A:305:TYR:O	3:A:409:EDO:H22	2.21	0.41
1:A:345:VAL:HB	4:A:427:ACT:H2	2.02	0.40
1:B:205[A]:GLU:HG3	3:B:409:EDO:H12	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/256 (99%)	249 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	257/256 (100%)	252 (98%)	5 (2%)	0	100	100
1	E	253/256 (99%)	246 (97%)	7 (3%)	0	100	100
1	G	252/256 (98%)	247 (98%)	4 (2%)	1 (0%)	30	28
1	I	243/256 (95%)	240 (99%)	3 (1%)	0	100	100
1	K	252/256 (98%)	243 (96%)	9 (4%)	0	100	100
All	All	1510/1536 (98%)	1477 (98%)	32 (2%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	332	ALA

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	224/224 (100%)	222 (99%)	2 (1%)	70	78
1	B	228/224 (102%)	227 (100%)	1 (0%)	84	89
1	E	224/224 (100%)	222 (99%)	2 (1%)	70	78
1	G	223/224 (100%)	221 (99%)	2 (1%)	70	78
1	I	222/224 (99%)	220 (99%)	2 (1%)	70	78
1	K	223/224 (100%)	220 (99%)	3 (1%)	61	69
All	All	1344/1344 (100%)	1332 (99%)	12 (1%)	70	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LEU
1	A	257	LYS
1	B	278	GLN
1	E	186	GLU
1	E	242	GLU

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Mol	Chain	Res	Type
1	K	184	ASN
1	K	200	LYS
1	K	241	ARG
1	G	310	LYS
1	G	334	GLU
1	I	123	THR
1	I	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	B	222	ASN
1	E	222	ASN
1	E	228	ASN
1	E	278	GLN
1	E	304	GLN
1	K	222	ASN
1	G	243	HIS
1	G	323	HIS
1	I	222	ASN
1	I	278	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

143 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	EDO	A	411	-	3,3,3	0.41	0	2,2,2	0.49	0
3	EDO	I	406	-	3,3,3	0.39	0	2,2,2	0.49	0
4	ACT	K	417	-	3,3,3	0.81	0	3,3,3	1.32	0
3	EDO	D	104	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	K	403	-	3,3,3	0.41	0	2,2,2	0.41	0
3	EDO	K	408	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	D	102	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	A	422	-	3,3,3	0.42	0	2,2,2	0.29	0
4	ACT	I	419	-	3,3,3	0.76	0	3,3,3	1.26	0
3	EDO	D	103	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	E	420	-	3,3,3	0.42	0	2,2,2	0.40	0
4	ACT	G	413	-	3,3,3	0.80	0	3,3,3	1.36	0
4	ACT	E	423	-	3,3,3	0.82	0	3,3,3	1.34	0
3	EDO	A	408	-	3,3,3	0.41	0	2,2,2	0.43	0
3	EDO	E	410	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	E	418	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	E	401	-	3,3,3	0.48	0	2,2,2	0.34	0
4	ACT	K	415	-	3,3,3	0.83	0	3,3,3	1.38	0
3	EDO	I	413	-	3,3,3	0.44	0	2,2,2	0.37	0
4	ACT	B	425	-	3,3,3	0.80	0	3,3,3	1.37	0
4	ACT	I	418	-	3,3,3	0.81	0	3,3,3	1.31	0
3	EDO	E	402	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	I	403	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	A	415	-	3,3,3	0.43	0	2,2,2	0.43	0
4	ACT	A	426	-	3,3,3	0.81	0	3,3,3	1.40	0
3	EDO	G	408	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	E	413	-	3,3,3	0.43	0	2,2,2	0.38	0
4	ACT	B	424	-	3,3,3	0.81	0	3,3,3	1.36	0
3	EDO	A	418[B]	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	E	408	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.42	0
4	ACT	A	424	-	3,3,3	0.78	0	3,3,3	1.14	0
3	EDO	E	417	-	3,3,3	0.44	0	2,2,2	0.26	0
3	EDO	F	102	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	A	421	-	3,3,3	0.44	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	K	409	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	B	417	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	I	409	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	K	410	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	J	102	-	3,3,3	0.44	0	2,2,2	0.32	0
4	ACT	E	422	-	3,3,3	0.80	0	3,3,3	1.30	0
4	ACT	I	417	-	3,3,3	0.80	0	3,3,3	1.21	0
3	EDO	E	412	-	3,3,3	0.41	0	2,2,2	0.40	0
4	ACT	E	424	-	3,3,3	0.77	0	3,3,3	1.42	0
3	EDO	B	422	-	3,3,3	0.45	0	2,2,2	0.27	0
3	EDO	E	409	-	3,3,3	0.41	0	2,2,2	0.43	0
3	EDO	A	409	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	A	410	-	3,3,3	0.43	0	2,2,2	0.37	0
5	6AH	D	101	2	7,7,7	0.47	0	6,6,6	0.72	0
4	ACT	A	423	-	3,3,3	0.83	0	3,3,3	1.27	0
3	EDO	I	414	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	K	401	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	B	408	-	3,3,3	0.42	0	2,2,2	0.44	0
4	ACT	E	421	-	3,3,3	0.80	0	3,3,3	1.21	0
3	EDO	I	412	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	G	411	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	I	416	-	3,3,3	0.40	0	2,2,2	0.44	0
3	EDO	I	411	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	G	405	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	A	418[A]	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	E	414	-	3,3,3	0.36	0	2,2,2	0.42	0
3	EDO	G	407	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	K	407	-	3,3,3	0.40	0	2,2,2	0.50	0
5	6AH	H	101	2	4,4,7	0.46	0	3,3,6	0.43	0
4	ACT	G	414	-	3,3,3	0.82	0	3,3,3	1.42	0
3	EDO	I	408[A]	-	3,3,3	0.44	0	2,2,2	0.36	0
5	6AH	F	101	2	7,7,7	0.49	0	6,6,6	0.67	0
4	ACT	B	423	-	3,3,3	0.76	0	3,3,3	1.34	0
4	ACT	A	427	-	3,3,3	0.90	0	3,3,3	1.12	0
3	EDO	B	410	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	I	408[B]	-	3,3,3	0.43	0	2,2,2	0.28	0
3	EDO	G	402	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	A	401	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	K	412	-	3,3,3	0.45	0	2,2,2	0.26	0
3	EDO	I	402	-	3,3,3	0.42	0	2,2,2	0.41	0
4	ACT	G	412	-	3,3,3	0.83	0	3,3,3	1.36	0
3	EDO	B	413	-	3,3,3	0.45	0	2,2,2	0.30	0
4	ACT	A	425	-	3,3,3	0.76	0	3,3,3	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	E	407	-	3,3,3	0.41	0	2,2,2	0.41	0
3	EDO	A	416	-	3,3,3	0.44	0	2,2,2	0.33	0
5	6AH	L	101	2	7,7,7	0.47	0	6,6,6	0.64	0
3	EDO	B	419	-	3,3,3	0.38	0	2,2,2	0.46	0
3	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.56	0
5	6AH	C	101	2	7,7,7	0.46	0	6,6,6	0.64	0
3	EDO	B	402	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	I	401	-	3,3,3	0.42	0	2,2,2	0.42	0
3	EDO	G	401	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	B	415	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	B	418	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	G	409	-	3,3,3	0.40	0	2,2,2	0.36	0
3	EDO	E	404	-	3,3,3	0.41	0	2,2,2	0.45	0
3	EDO	A	404	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	B	403	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	416	-	3,3,3	0.44	0	2,2,2	0.35	0
4	ACT	I	420	-	3,3,3	0.79	0	3,3,3	1.39	0
3	EDO	B	401	-	3,3,3	0.43	0	2,2,2	0.30	0
3	EDO	K	405	-	3,3,3	0.38	0	2,2,2	0.53	0
3	EDO	B	411	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	B	421	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	G	410	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	A	405	-	3,3,3	0.41	0	2,2,2	0.43	0
3	EDO	B	406	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	A	402	-	3,3,3	0.36	0	2,2,2	0.52	0
3	EDO	E	406	-	3,3,3	0.47	0	2,2,2	0.25	0
3	EDO	H	104	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	A	406	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	B	420	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	K	404	-	3,3,3	0.41	0	2,2,2	0.47	0
3	EDO	A	407	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	B	412	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	I	410	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	A	412	-	3,3,3	0.40	0	2,2,2	0.11	0
3	EDO	E	416	-	3,3,3	0.53	0	2,2,2	0.22	0
3	EDO	I	404	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	G	404	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	G	403	-	3,3,3	0.40	0	2,2,2	0.45	0
3	EDO	E	405	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	H	103	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	E	419	-	3,3,3	0.42	0	2,2,2	0.39	0
4	ACT	K	416	-	3,3,3	0.83	0	3,3,3	1.39	0
3	EDO	E	415	-	3,3,3	0.45	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	K	406	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	A	417	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	A	420	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	B	414	-	3,3,3	0.45	0	2,2,2	0.31	0
5	6AH	J	101	2	7,7,7	0.48	0	6,6,6	0.68	0
3	EDO	K	413	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	A	414	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	I	405	-	3,3,3	0.48	0	2,2,2	0.25	0
3	EDO	G	406	-	3,3,3	0.41	0	2,2,2	0.49	0
3	EDO	I	407	-	3,3,3	0.40	0	2,2,2	0.42	0
3	EDO	B	409	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	I	415	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	413	-	3,3,3	0.41	0	2,2,2	0.46	0
3	EDO	E	403	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.41	0
3	EDO	K	411	-	3,3,3	0.42	0	2,2,2	0.41	0
3	EDO	H	102	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	A	419	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	E	411	-	3,3,3	0.40	0	2,2,2	0.37	0
3	EDO	K	414	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	K	402	-	3,3,3	0.41	0	2,2,2	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	411	-	-	0/1/1/1	-
3	EDO	I	406	-	-	0/1/1/1	-
3	EDO	D	104	-	-	0/1/1/1	-
3	EDO	K	403	-	-	0/1/1/1	-
3	EDO	K	408	-	-	0/1/1/1	-
3	EDO	D	102	-	-	1/1/1/1	-
3	EDO	A	422	-	-	0/1/1/1	-
3	EDO	D	103	-	-	0/1/1/1	-
3	EDO	E	420	-	-	0/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-
3	EDO	E	410	-	-	0/1/1/1	-
3	EDO	E	418	-	-	0/1/1/1	-
3	EDO	E	401	-	-	0/1/1/1	-
3	EDO	I	413	-	-	0/1/1/1	-
3	EDO	E	402	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	I	403	-	-	0/1/1/1	-
3	EDO	A	415	-	-	0/1/1/1	-
3	EDO	G	408	-	-	0/1/1/1	-
3	EDO	E	413	-	-	0/1/1/1	-
3	EDO	A	418[B]	-	-	1/1/1/1	-
3	EDO	E	408	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
3	EDO	E	417	-	-	0/1/1/1	-
3	EDO	F	102	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	421	-	-	0/1/1/1	-
3	EDO	K	409	-	-	0/1/1/1	-
3	EDO	B	417	-	-	0/1/1/1	-
3	EDO	I	409	-	-	0/1/1/1	-
3	EDO	K	410	-	-	0/1/1/1	-
3	EDO	J	102	-	-	0/1/1/1	-
3	EDO	E	412	-	-	0/1/1/1	-
3	EDO	B	422	-	-	0/1/1/1	-
3	EDO	E	409	-	-	0/1/1/1	-
3	EDO	A	409	-	-	0/1/1/1	-
3	EDO	A	410	-	-	0/1/1/1	-
5	6AH	D	101	2	-	2/5/5/5	-
3	EDO	I	414	-	-	0/1/1/1	-
3	EDO	K	401	-	-	0/1/1/1	-
3	EDO	B	408	-	-	0/1/1/1	-
3	EDO	I	412	-	-	0/1/1/1	-
3	EDO	G	411	-	-	0/1/1/1	-
3	EDO	I	416	-	-	0/1/1/1	-
3	EDO	I	411	-	-	1/1/1/1	-
3	EDO	G	405	-	-	0/1/1/1	-
3	EDO	A	418[A]	-	-	0/1/1/1	-
3	EDO	E	414	-	-	0/1/1/1	-
3	EDO	G	407	-	-	0/1/1/1	-
3	EDO	K	407	-	-	0/1/1/1	-
5	6AH	H	101	2	-	1/2/2/5	-
3	EDO	I	408[A]	-	-	0/1/1/1	-
5	6AH	F	101	2	-	4/5/5/5	-
3	EDO	B	410	-	-	0/1/1/1	-
3	EDO	I	408[B]	-	-	0/1/1/1	-
3	EDO	G	402	-	-	0/1/1/1	-
3	EDO	A	401	-	-	1/1/1/1	-
3	EDO	K	412	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	I	402	-	-	0/1/1/1	-
3	EDO	B	413	-	-	0/1/1/1	-
3	EDO	E	407	-	-	0/1/1/1	-
3	EDO	A	416	-	-	0/1/1/1	-
5	6AH	L	101	2	-	1/5/5/5	-
3	EDO	B	419	-	-	0/1/1/1	-
3	EDO	B	405	-	-	0/1/1/1	-
5	6AH	C	101	2	-	3/5/5/5	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	I	401	-	-	0/1/1/1	-
3	EDO	G	401	-	-	0/1/1/1	-
3	EDO	B	415	-	-	0/1/1/1	-
3	EDO	B	418	-	-	0/1/1/1	-
3	EDO	G	409	-	-	0/1/1/1	-
3	EDO	E	404	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	B	416	-	-	1/1/1/1	-
3	EDO	B	401	-	-	1/1/1/1	-
3	EDO	K	405	-	-	1/1/1/1	-
3	EDO	B	411	-	-	0/1/1/1	-
3	EDO	B	421	-	-	0/1/1/1	-
3	EDO	G	410	-	-	0/1/1/1	-
3	EDO	A	405	-	-	0/1/1/1	-
3	EDO	B	406	-	-	0/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	E	406	-	-	0/1/1/1	-
3	EDO	H	104	-	-	0/1/1/1	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	B	420	-	-	0/1/1/1	-
3	EDO	K	404	-	-	0/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	B	412	-	-	0/1/1/1	-
3	EDO	I	410	-	-	1/1/1/1	-
3	EDO	A	412	-	-	0/1/1/1	-
3	EDO	E	416	-	-	0/1/1/1	-
3	EDO	I	404	-	-	0/1/1/1	-
3	EDO	G	404	-	-	0/1/1/1	-
3	EDO	G	403	-	-	0/1/1/1	-
3	EDO	E	405	-	-	0/1/1/1	-
3	EDO	H	103	-	-	0/1/1/1	-
3	EDO	E	419	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	415	-	-	1/1/1/1	-
3	EDO	K	406	-	-	0/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-
3	EDO	A	420	-	-	0/1/1/1	-
3	EDO	B	414	-	-	0/1/1/1	-
5	6AH	J	101	2	-	3/5/5/5	-
3	EDO	K	413	-	-	0/1/1/1	-
3	EDO	A	414	-	-	0/1/1/1	-
3	EDO	I	405	-	-	0/1/1/1	-
3	EDO	G	406	-	-	0/1/1/1	-
3	EDO	I	407	-	-	1/1/1/1	-
3	EDO	B	409	-	-	0/1/1/1	-
3	EDO	I	415	-	-	0/1/1/1	-
3	EDO	A	413	-	-	0/1/1/1	-
3	EDO	E	403	-	-	0/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	K	411	-	-	0/1/1/1	-
3	EDO	H	102	-	-	0/1/1/1	-
3	EDO	A	419	-	-	0/1/1/1	-
3	EDO	E	411	-	-	0/1/1/1	-
3	EDO	K	414	-	-	0/1/1/1	-
3	EDO	K	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	101	6AH	C1-C2-C3-C4
5	F	101	6AH	C1-C2-C3-C4
5	D	101	6AH	C1-C2-C3-C4
5	H	101	6AH	C1-C2-C3-C4
5	F	101	6AH	C2-C3-C4-C5
5	C	101	6AH	O-C1-C2-C3
5	D	101	6AH	O-C1-C2-C3
5	F	101	6AH	O-C1-C2-C3
5	F	101	6AH	C3-C4-C5-C6
3	A	401	EDO	O1-C1-C2-O2
5	C	101	6AH	C1-C2-C3-C4
5	J	101	6AH	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	J	101	6AH	O-C1-C2-C3
3	B	401	EDO	O1-C1-C2-O2
3	E	415	EDO	O1-C1-C2-O2
5	C	101	6AH	C2-C3-C4-C5
3	A	402	EDO	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
3	B	416	EDO	O1-C1-C2-O2
3	D	102	EDO	O1-C1-C2-O2
3	K	405	EDO	O1-C1-C2-O2
3	I	410	EDO	O1-C1-C2-O2
3	I	407	EDO	O1-C1-C2-O2
5	J	101	6AH	C1-C2-C3-C4
3	A	418[B]	EDO	O1-C1-C2-O2
3	I	411	EDO	O1-C1-C2-O2

There are no ring outliers.

36 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	104	EDO	1	0
3	K	408	EDO	1	0
3	D	103	EDO	1	0
3	E	420	EDO	1	0
4	I	418	ACT	1	0
3	F	102	EDO	1	0
3	A	421	EDO	1	0
3	B	417	EDO	1	0
3	A	409	EDO	2	0
3	K	401	EDO	1	0
3	I	412	EDO	1	0
3	I	416	EDO	2	0
3	G	405	EDO	1	0
3	E	414	EDO	2	0
3	K	407	EDO	1	0
4	G	414	ACT	1	0
5	F	101	6AH	1	0
4	B	423	ACT	1	0
4	A	427	ACT	1	0
3	A	401	EDO	2	0
3	B	419	EDO	1	0
3	E	404	EDO	1	0
3	B	403	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	416	EDO	1	0
3	B	401	EDO	1	0
3	K	405	EDO	1	0
3	A	405	EDO	1	0
3	E	406	EDO	1	0
3	A	412	EDO	1	0
3	I	404	EDO	1	0
3	G	404	EDO	1	0
3	E	415	EDO	3	0
3	I	405	EDO	1	0
3	B	409	EDO	1	0
3	I	415	EDO	1	0
3	K	414	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	250/256 (97%)	-0.41	2 (0%) 82 85	19, 33, 61, 84	5 (2%)
1	B	250/256 (97%)	-0.34	3 (1%) 76 79	17, 37, 68, 107	9 (3%)
1	E	250/256 (97%)	-0.61	0 100 100	20, 32, 52, 72	5 (2%)
1	G	249/256 (97%)	-0.23	4 (1%) 70 73	21, 40, 80, 115	5 (2%)
1	I	250/256 (97%)	-0.27	4 (1%) 70 73	20, 39, 75, 111	3 (1%)
1	K	249/256 (97%)	-0.10	3 (1%) 76 79	24, 48, 94, 137	5 (2%)
2	C	9/9 (100%)	-0.39	0 100 100	41, 61, 76, 77	0
2	D	9/9 (100%)	-0.58	0 100 100	32, 51, 73, 78	0
2	F	9/9 (100%)	-0.24	0 100 100	34, 58, 83, 92	0
2	H	9/9 (100%)	-0.66	0 100 100	34, 45, 61, 68	0
2	J	9/9 (100%)	-0.39	0 100 100	44, 60, 74, 82	0
2	L	9/9 (100%)	-0.26	0 100 100	43, 61, 71, 74	0
All	All	1552/1590 (97%)	-0.33	16 (1%) 79 82	17, 38, 75, 137	32 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	332	ALA	4.7
1	G	370	LEU	3.1
1	I	370	LEU	3.1
1	K	370	LEU	2.9
1	A	122	SER	2.9
1	G	170	TYR	2.8
1	K	316[A]	ARG	2.8
1	I	283	CYS	2.5
1	I	262	PRO	2.5
1	K	225	LEU	2.4
1	I	121	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	122	SER	2.2
1	A	197	GLY	2.1
1	B	370	LEU	2.1
1	B	226	GLY	2.1
1	G	333	GLU	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	EDO	K	411	4/4	0.68	0.14	87,87,88,89	0
4	ACT	G	412	4/4	0.70	0.21	80,80,81,81	0
3	EDO	G	404	4/4	0.72	0.19	84,87,89,90	0
3	EDO	B	421	4/4	0.73	0.22	95,96,99,101	0
3	EDO	G	406	4/4	0.74	0.17	80,80,81,83	0
3	EDO	K	414	4/4	0.76	0.18	58,64,69,70	0
3	EDO	G	410	4/4	0.77	0.20	88,89,91,93	0
4	ACT	E	423	4/4	0.77	0.17	77,82,84,85	0
3	EDO	B	418	4/4	0.77	0.17	81,82,83,84	0
4	ACT	I	420	4/4	0.77	0.27	82,84,86,86	0
3	EDO	B	417	4/4	0.78	0.26	95,95,95,98	0
3	EDO	B	406	4/4	0.78	0.19	84,85,85,86	0
3	EDO	I	414	4/4	0.78	0.27	62,70,76,81	0
3	EDO	I	412	4/4	0.79	0.20	91,91,92,92	0
3	EDO	E	408	4/4	0.79	0.17	87,88,92,95	0
3	EDO	A	416	4/4	0.79	0.15	71,72,74,75	0
3	EDO	D	103	4/4	0.79	0.24	66,69,71,72	0
3	EDO	G	411	4/4	0.79	0.21	75,76,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	426	4/4	0.80	0.17	75,78,79,82	0
3	EDO	H	104	4/4	0.80	0.19	68,74,77,77	0
3	EDO	A	417	4/4	0.80	0.19	79,79,80,82	0
3	EDO	G	402	4/4	0.80	0.14	80,81,81,81	0
4	ACT	G	414	4/4	0.81	0.20	73,73,73,75	0
4	ACT	A	427	4/4	0.82	0.22	51,56,60,65	0
3	EDO	K	410	4/4	0.82	0.26	93,95,96,96	0
3	EDO	B	420	4/4	0.82	0.22	91,92,93,94	0
3	EDO	B	419	4/4	0.82	0.30	56,61,68,74	0
3	EDO	E	418	4/4	0.82	0.18	90,92,94,95	0
3	EDO	I	408[A]	4/4	0.83	0.19	53,55,55,57	4
4	ACT	E	421	4/4	0.83	0.14	40,57,61,76	0
3	EDO	I	408[B]	4/4	0.83	0.19	51,54,57,58	4
3	EDO	K	412	4/4	0.83	0.19	50,57,62,65	0
3	EDO	H	102	4/4	0.83	0.20	64,68,72,76	0
3	EDO	E	415	4/4	0.83	0.17	44,48,54,64	0
3	EDO	G	408	4/4	0.84	0.16	79,83,84,84	0
3	EDO	E	416	4/4	0.84	0.14	37,38,45,47	0
3	EDO	B	403	4/4	0.84	0.17	53,54,57,69	0
4	ACT	I	419	4/4	0.84	0.23	68,74,76,82	0
3	EDO	B	411	4/4	0.84	0.14	69,71,71,71	0
3	EDO	I	406	4/4	0.85	0.17	71,72,75,76	0
3	EDO	B	405	4/4	0.85	0.23	59,59,61,63	0
3	EDO	B	410	4/4	0.85	0.22	76,77,79,80	0
4	ACT	B	423	4/4	0.85	0.18	64,65,71,81	0
3	EDO	E	412	4/4	0.85	0.18	47,64,71,79	0
3	EDO	D	104	4/4	0.86	0.18	70,71,73,74	0
3	EDO	E	403	4/4	0.86	0.25	81,84,89,90	0
3	EDO	E	413	4/4	0.86	0.15	63,65,70,74	0
3	EDO	K	413	4/4	0.86	0.23	73,75,77,81	0
3	EDO	I	409	4/4	0.86	0.15	41,51,51,52	0
4	ACT	K	415	4/4	0.86	0.14	57,63,64,73	0
3	EDO	K	407	4/4	0.86	0.18	71,71,74,74	0
4	ACT	G	413	4/4	0.86	0.18	88,89,90,90	0
3	EDO	K	409	4/4	0.86	0.23	74,78,81,86	0
4	ACT	I	417	4/4	0.86	0.14	48,51,58,60	0
4	ACT	I	418	4/4	0.86	0.15	52,65,66,68	0
4	ACT	A	424	4/4	0.86	0.18	48,54,57,62	0
4	ACT	A	425	4/4	0.86	0.17	62,65,65,66	0
3	EDO	A	419	4/4	0.87	0.18	85,88,90,90	0
3	EDO	B	422	4/4	0.87	0.14	75,75,77,80	0
3	EDO	E	419	4/4	0.87	0.17	80,80,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	E	420	4/4	0.87	0.14	73,75,75,75	0
3	EDO	I	413	4/4	0.87	0.18	75,75,76,79	0
4	ACT	B	424	4/4	0.87	0.16	73,77,78,80	0
3	EDO	A	415	4/4	0.87	0.16	62,68,72,73	0
3	EDO	J	102	4/4	0.87	0.20	78,79,80,80	0
3	EDO	A	402	4/4	0.88	0.14	50,51,56,58	0
3	EDO	E	407	4/4	0.88	0.16	68,69,74,78	0
3	EDO	I	404	4/4	0.88	0.14	42,50,57,61	0
3	EDO	B	416	4/4	0.88	0.14	69,73,78,80	0
3	EDO	I	407	4/4	0.88	0.21	65,68,71,81	0
3	EDO	E	410	4/4	0.88	0.16	72,74,75,75	0
3	EDO	K	402	4/4	0.88	0.13	55,59,59,61	0
3	EDO	G	403	4/4	0.88	0.22	66,67,68,73	0
3	EDO	K	404	4/4	0.88	0.16	57,64,65,69	0
3	EDO	K	405	4/4	0.88	0.14	41,41,49,56	0
3	EDO	A	407	4/4	0.88	0.14	53,59,66,69	0
3	EDO	I	415	4/4	0.88	0.11	79,79,80,80	0
3	EDO	I	416	4/4	0.88	0.13	61,67,73,75	0
3	EDO	A	410	4/4	0.88	0.15	80,82,83,86	0
3	EDO	A	411	4/4	0.88	0.26	72,73,77,78	0
4	ACT	K	417	4/4	0.89	0.12	72,78,79,81	0
3	EDO	A	413	4/4	0.89	0.14	54,58,65,70	0
3	EDO	E	417	4/4	0.89	0.17	69,72,72,73	0
4	ACT	B	425	4/4	0.89	0.13	75,79,80,83	0
3	EDO	A	414	4/4	0.89	0.19	81,81,85,89	0
3	EDO	G	407	4/4	0.89	0.25	60,62,62,63	0
3	EDO	A	421	4/4	0.89	0.16	76,77,77,79	0
4	ACT	K	416	4/4	0.89	0.16	63,65,67,72	0
5	6AH	L	101	8/8	0.89	0.23	64,81,100,101	0
3	EDO	I	401	4/4	0.90	0.12	51,56,65,68	0
3	EDO	I	403	4/4	0.90	0.17	40,42,46,48	0
3	EDO	A	420	4/4	0.90	0.14	91,93,95,95	0
3	EDO	I	405	4/4	0.90	0.14	58,58,59,63	0
3	EDO	A	418[A]	4/4	0.90	0.17	27,27,35,38	4
3	EDO	A	418[B]	4/4	0.90	0.17	32,38,39,43	4
3	EDO	B	413	4/4	0.90	0.17	58,66,68,71	0
3	EDO	B	415	4/4	0.90	0.12	48,57,62,65	0
3	EDO	A	401	4/4	0.90	0.13	38,49,54,61	0
3	EDO	I	410	4/4	0.90	0.14	57,58,58,59	0
3	EDO	H	103	4/4	0.90	0.22	76,77,80,82	0
3	EDO	E	411	4/4	0.90	0.14	71,72,73,77	0
3	EDO	E	414	4/4	0.91	0.18	41,53,60,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	404	4/4	0.91	0.14	66,67,67,71	0
3	EDO	E	405	4/4	0.91	0.21	41,51,54,56	0
3	EDO	K	403	4/4	0.91	0.14	63,65,66,66	0
3	EDO	B	408	4/4	0.91	0.17	72,75,75,79	0
3	EDO	A	408	4/4	0.91	0.16	46,48,50,63	0
3	EDO	A	409	4/4	0.92	0.13	42,47,49,49	0
3	EDO	K	406	4/4	0.92	0.19	75,77,85,89	0
3	EDO	B	412	4/4	0.92	0.12	53,58,64,71	0
3	EDO	B	409	4/4	0.92	0.13	61,62,68,71	0
3	EDO	F	102	4/4	0.92	0.16	69,70,74,75	0
3	EDO	E	409	4/4	0.92	0.18	55,57,58,62	0
3	EDO	B	414	4/4	0.92	0.14	50,62,69,70	0
3	EDO	B	407	4/4	0.92	0.15	72,73,77,77	0
3	EDO	E	406	4/4	0.93	0.13	45,53,58,59	0
3	EDO	A	404	4/4	0.93	0.10	39,40,45,53	0
4	ACT	E	422	4/4	0.93	0.15	77,78,78,79	0
3	EDO	K	408	4/4	0.93	0.17	44,50,55,61	0
4	ACT	E	424	4/4	0.93	0.12	44,57,63,66	0
3	EDO	A	403	4/4	0.93	0.11	42,56,60,64	0
3	EDO	A	422	4/4	0.93	0.17	55,56,60,60	0
5	6AH	F	101	8/8	0.93	0.14	44,54,57,60	0
3	EDO	I	411	4/4	0.93	0.14	49,49,54,58	0
3	EDO	G	405	4/4	0.94	0.16	41,50,51,54	0
3	EDO	G	401	4/4	0.94	0.08	43,43,45,46	0
3	EDO	A	405	4/4	0.94	0.12	52,53,60,67	0
3	EDO	A	406	4/4	0.94	0.14	70,71,77,81	0
4	ACT	A	423	4/4	0.94	0.14	53,65,66,71	0
3	EDO	D	102	4/4	0.94	0.16	82,85,88,89	0
3	EDO	I	402	4/4	0.94	0.11	48,50,54,57	0
5	6AH	H	101	5/8	0.94	0.14	41,47,58,60	0
5	6AH	J	101	8/8	0.94	0.15	54,69,79,80	0
3	EDO	E	402	4/4	0.95	0.10	29,33,34,38	0
5	6AH	C	101	8/8	0.95	0.12	49,56,61,63	0
3	EDO	E	404	4/4	0.95	0.10	38,43,52,58	0
3	EDO	B	402	4/4	0.96	0.07	43,43,50,58	0
5	6AH	D	101	8/8	0.96	0.09	38,44,47,50	0
3	EDO	A	412	4/4	0.96	0.11	30,34,41,42	0
3	EDO	B	401	4/4	0.97	0.09	32,35,35,36	0
3	EDO	E	401	4/4	0.97	0.06	30,32,34,35	0
3	EDO	K	401	4/4	0.97	0.07	33,38,40,47	0
3	EDO	G	409	4/4	0.98	0.06	27,36,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.