



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2017 – 10:56 AM EDT

PDB ID : 5T7O
Title : Crystal structure of Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase in complex with (6S)-5,6,7,8-TETRAHYDROFOLATE
Authors : Di Pisa, F.; Dello Iacono, L.; Bonucci, A.; Mangani, S.
Deposited on : unknown
Resolution : 1.80 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

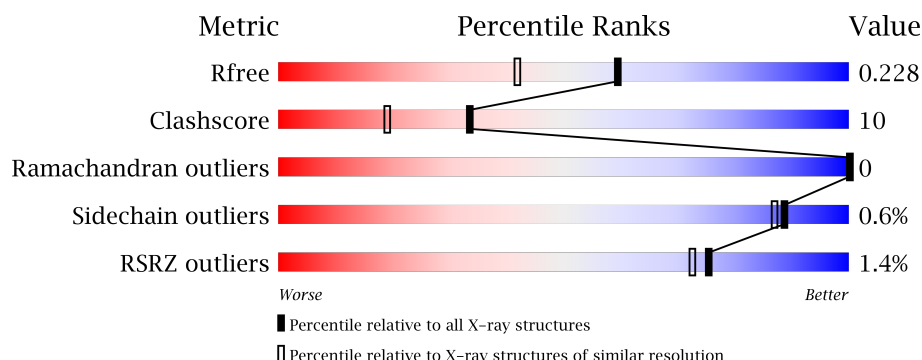
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	521	
1	B	521	
1	C	521	
1	D	521	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	THG	D	703	-	-	-	X
4	UMP	A	703	-	-	-	X
4	UMP	B	602	-	-	-	X
4	UMP	C	603	-	-	-	X
4	UMP	D	702	-	-	-	X
5	EDO	A	707	-	-	-	X
5	EDO	A	711	-	-	-	X
5	EDO	A	714	-	-	-	X
5	EDO	B	606	-	-	-	X
5	EDO	B	607	-	-	-	X
5	EDO	B	608	-	-	-	X
5	EDO	B	609	-	-	-	X
5	EDO	B	611	-	-	-	X
5	EDO	B	612	-	-	-	X
5	EDO	B	613	-	-	-	X
5	EDO	C	606	-	-	-	X
5	EDO	C	607	-	-	-	X
5	EDO	C	608	-	-	-	X
5	EDO	C	609	-	-	-	X
5	EDO	C	610	-	-	-	X
5	EDO	C	611	-	-	-	X
5	EDO	C	613	-	-	-	X
5	EDO	C	614	-	-	-	X
5	EDO	D	705	-	-	-	X
5	EDO	D	708	-	-	-	X
5	EDO	D	710	-	-	-	X
5	EDO	D	712	-	-	-	X
5	EDO	D	713	-	-	-	X

2 Entry composition ⓘ

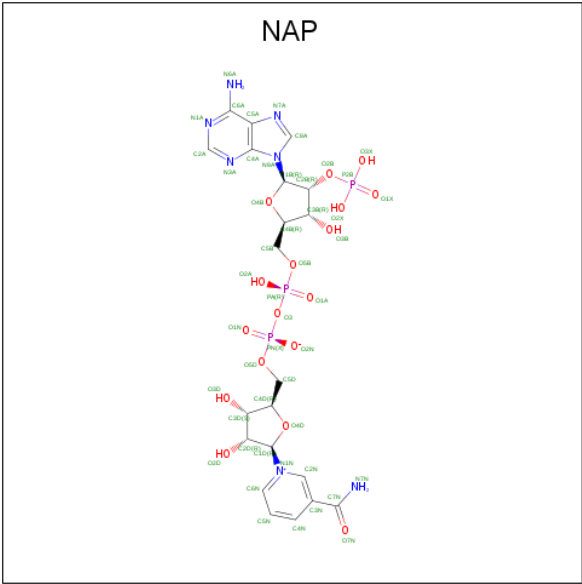
There are 6 unique types of molecules in this entry. The entry contains 18488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	25	0
			4003	2563	698	720	22			
1	B	495	Total	C	N	O	S	0	21	0
			4017	2572	701	722	22			
1	C	487	Total	C	N	O	S	0	23	0
			3947	2531	689	707	20			
1	D	489	Total	C	N	O	S	0	13	0
			3909	2501	684	707	17			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



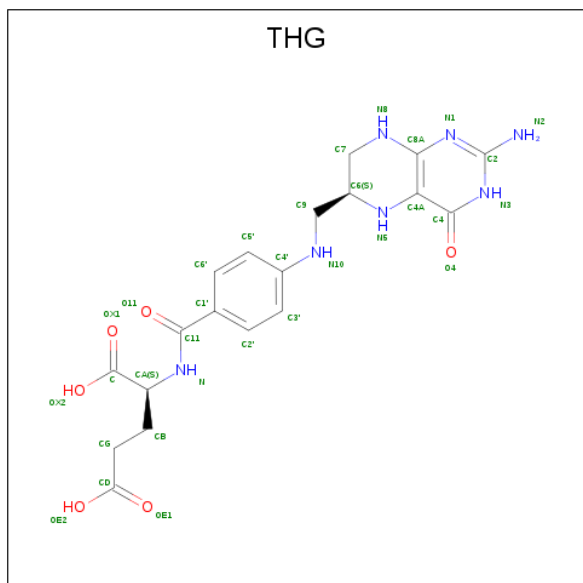
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

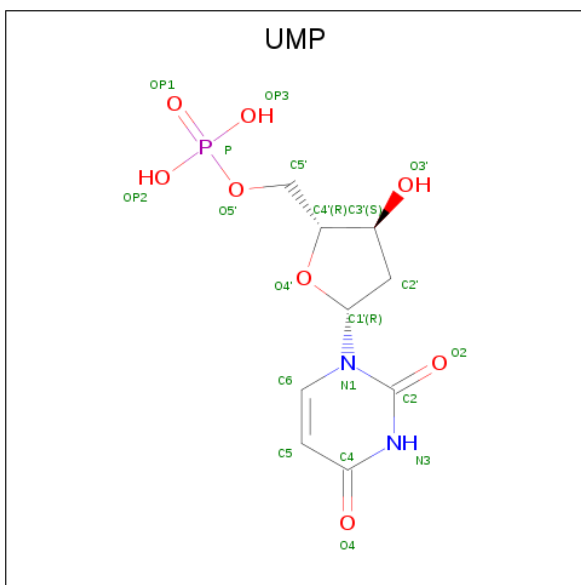
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	D	1	Total	C	N	O	P	0
			48	21	7	17	3	

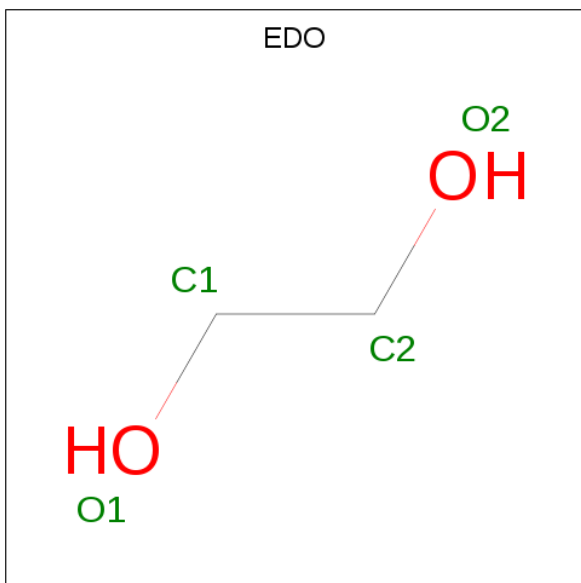
- Molecule 3 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
4	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
4	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
4	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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



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

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

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

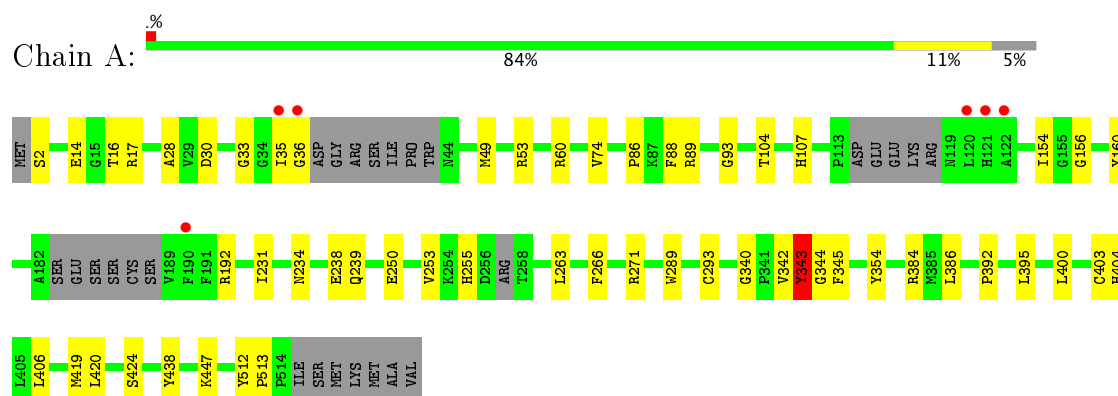
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	527	Total 527	O 527	0	0
6	B	514	Total 514	O 514	0	4
6	C	518	Total 518	O 518	0	1
6	D	465	Total 465	O 465	0	0

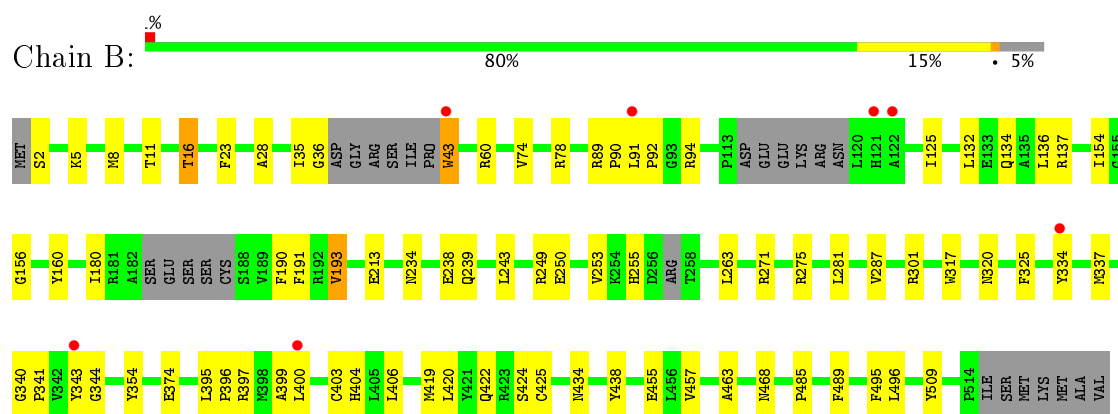
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

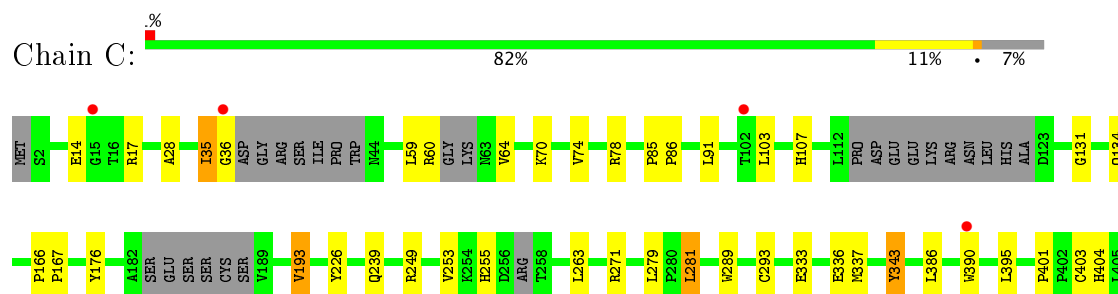
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

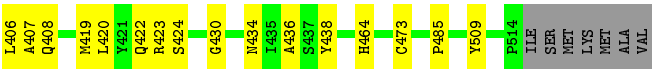


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

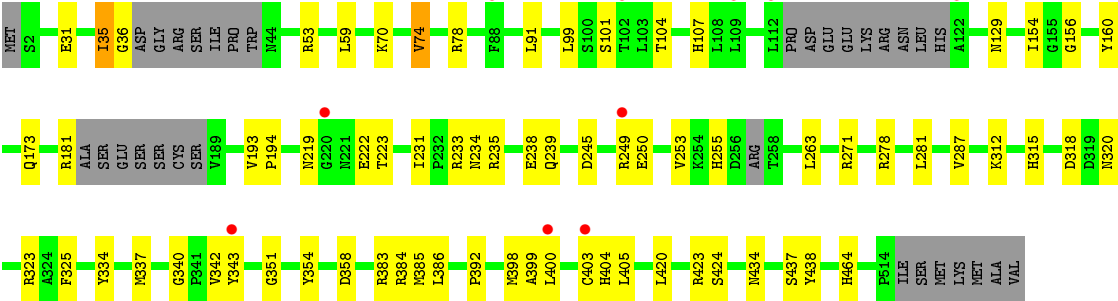
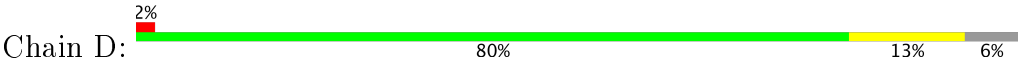


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





● Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.55Å 173.54Å 174.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.77 – 1.80 69.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.77-1.80) 99.2 (69.51-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.220 0.188 , 0.228	Depositor DCC
R_{free} test set	10547 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0996e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.24	2/4161 (0.0%)	1.08	4/5648 (0.1%)
1	B	1.23	0/4169	1.07	0/5659
1	C	1.25	1/4092 (0.0%)	1.12	3/5550 (0.1%)
1	D	1.23	1/4027 (0.0%)	1.08	2/5467 (0.0%)
All	All	1.24	4/16449 (0.0%)	1.09	9/22324 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	343	TYR	CB-CG	19.02	1.80	1.51
1	D	385	MET	C-N	-8.31	1.15	1.34
1	A	344	GLY	N-CA	6.48	1.55	1.46
1	A	344	GLY	CA-C	-5.03	1.43	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	TYR	CA-CB-CG	-6.66	100.75	113.40
1	C	343	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	343	TYR	CB-CG-CD1	6.38	124.83	121.00
1	A	400	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	74[A]	VAL	CB-CA-C	5.39	121.65	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	TYR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4003	0	3985	65	0
1	B	4017	0	3996	99	0
1	C	3947	0	3957	72	0
1	D	3909	0	3857	82	0
2	A	48	0	25	5	0
2	B	48	0	25	11	0
2	C	48	0	25	3	0
2	D	48	0	25	8	0
3	A	32	0	21	3	0
3	B	32	0	21	2	0
3	C	32	0	21	1	0
3	D	32	0	21	3	0
4	A	20	0	11	4	0
4	B	20	0	11	3	0
4	C	20	0	11	5	0
4	D	20	0	11	2	0
5	A	56	0	84	5	0
5	B	48	0	72	8	0
5	C	44	0	66	9	0
5	D	40	0	60	3	0
6	A	527	0	0	12	0
6	B	514	0	0	20	0
6	C	518	0	0	9	0
6	D	465	0	0	15	0
All	All	18488	0	16305	319	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 10.

The worst 5 of 319 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:343:TYR:CB	1:C:343:TYR:CG	1.80	1.64
1:B:337:MET:HG3	6:B:1142:HOH:O	1.42	1.19
1:B:8[B]:MET:CE	1:B:496:LEU:N	2.07	1.15
1:D:337:MET:HG3	6:D:1228:HOH:O	1.47	1.15
6:C:1040:HOH:O	1:D:400:LEU:HD23	1.50	1.11

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	508/521 (98%)	494 (97%)	14 (3%)	0	100	100
1	B	506/521 (97%)	495 (98%)	11 (2%)	0	100	100
1	C	497/521 (95%)	485 (98%)	12 (2%)	0	100	100
1	D	491/521 (94%)	474 (96%)	17 (4%)	0	100	100
All	All	2002/2084 (96%)	1948 (97%)	54 (3%)	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	429/446 (96%)	428 (100%)	1 (0%)	94	93
1	B	431/446 (97%)	425 (99%)	6 (1%)	71	64
1	C	424/446 (95%)	418 (99%)	6 (1%)	71	64
1	D	413/446 (93%)	411 (100%)	2 (0%)	91	90
All	All	1697/1784 (95%)	1682 (99%)	15 (1%)	89	78

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

Mol	Chain	Res	Type
1	B	468	ASN
1	C	35[A]	ILE
1	C	281[C]	LEU
1	B	193[B]	VAL
1	C	281[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	143	ASN
1	C	356	HIS
1	D	315	HIS
1	C	239	GLN
1	C	379	ASN

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

59 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$
2	NAP	A	701	-	44,52,52	1.12	4 (9%)	51,80,80	1.96	8 (15%)
3	THG	A	702	-	25,34,34	2.10	6 (24%)	28,47,47	2.18	7 (25%)
4	UMP	A	703	-	17,21,21	1.07	1 (5%)	23,31,31	3.29	3 (13%)
5	EDO	A	704	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	705	-	3,3,3	0.58	0	2,2,2	0.80	0
5	EDO	A	706	-	3,3,3	0.67	0	2,2,2	0.81	0
5	EDO	A	707	-	3,3,3	0.46	0	2,2,2	0.82	0
5	EDO	A	708	-	3,3,3	0.40	0	2,2,2	0.40	0
5	EDO	A	709	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	710	-	3,3,3	0.55	0	2,2,2	0.77	0
5	EDO	A	711	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	712	-	3,3,3	0.43	0	2,2,2	0.48	0
5	EDO	A	713	-	3,3,3	0.96	0	2,2,2	0.50	0
5	EDO	A	714	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	715	-	3,3,3	0.49	0	2,2,2	0.76	0
5	EDO	A	716	-	3,3,3	0.47	0	2,2,2	1.22	0
5	EDO	A	717	-	3,3,3	0.47	0	2,2,2	0.81	0
3	THG	B	601	-	25,34,34	2.46	8 (32%)	28,47,47	2.37	7 (25%)
4	UMP	B	602	-	17,21,21	1.26	3 (17%)	23,31,31	3.34	4 (17%)
2	NAP	B	603	-	44,52,52	1.17	5 (11%)	51,80,80	1.78	11 (21%)
5	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	605	-	3,3,3	0.71	0	2,2,2	0.74	0
5	EDO	B	606	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	608	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	609	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	B	610	-	3,3,3	0.52	0	2,2,2	0.63	0
5	EDO	B	611	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	B	612	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	613	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	614	-	3,3,3	0.34	0	2,2,2	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	615	-	3,3,3	0.81	0	2,2,2	0.43	0
3	THG	C	601	-	25,34,34	1.95	4 (16%)	28,47,47	2.07	7 (25%)
2	NAP	C	602	-	44,52,52	1.20	5 (11%)	51,80,80	2.20	16 (31%)
4	UMP	C	603	-	17,21,21	1.07	1 (5%)	23,31,31	3.26	3 (13%)
5	EDO	C	604	-	3,3,3	0.69	0	2,2,2	0.41	0
5	EDO	C	605	-	3,3,3	0.34	0	2,2,2	0.84	0
5	EDO	C	606	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	C	607	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	608	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	609	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	C	610	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	C	611	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	C	612	-	3,3,3	0.85	0	2,2,2	0.71	0
5	EDO	C	613	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	614	-	3,3,3	0.45	0	2,2,2	0.37	0
2	NAP	D	701	-	44,52,52	1.09	4 (9%)	51,80,80	1.66	8 (15%)
4	UMP	D	702	-	17,21,21	1.06	1 (5%)	23,31,31	3.28	3 (13%)
3	THG	D	703	-	25,34,34	1.48	2 (8%)	28,47,47	1.39	3 (10%)
5	EDO	D	704	-	3,3,3	0.44	0	2,2,2	0.90	0
5	EDO	D	705	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	D	706	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	D	707	-	3,3,3	0.41	0	2,2,2	0.64	0
5	EDO	D	708	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	D	709	-	3,3,3	0.93	0	2,2,2	0.76	0
5	EDO	D	710	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	D	711	-	3,3,3	0.44	0	2,2,2	0.76	0
5	EDO	D	712	-	3,3,3	0.40	0	2,2,2	0.19	0
5	EDO	D	713	-	3,3,3	0.45	0	2,2,2	0.36	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
2	NAP	A	701	-	-	0/27/67/67	0/5/5/5
3	THG	A	702	-	-	0/16/31/31	0/3/3/3
4	UMP	A	703	-	-	0/6/22/22	0/2/2/2
5	EDO	A	704	-	-	0/1/1/1	0/0/0/0
5	EDO	A	705	-	-	0/1/1/1	0/0/0/0
5	EDO	A	706	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	707	-	-	0/1/1/1	0/0/0/0
5	EDO	A	708	-	-	0/1/1/1	0/0/0/0
5	EDO	A	709	-	-	0/1/1/1	0/0/0/0
5	EDO	A	710	-	-	0/1/1/1	0/0/0/0
5	EDO	A	711	-	-	0/1/1/1	0/0/0/0
5	EDO	A	712	-	-	0/1/1/1	0/0/0/0
5	EDO	A	713	-	-	0/1/1/1	0/0/0/0
5	EDO	A	714	-	-	0/1/1/1	0/0/0/0
5	EDO	A	715	-	-	0/1/1/1	0/0/0/0
5	EDO	A	716	-	-	0/1/1/1	0/0/0/0
5	EDO	A	717	-	-	0/1/1/1	0/0/0/0
3	THG	B	601	-	-	0/16/31/31	0/3/3/3
4	UMP	B	602	-	-	0/6/22/22	0/2/2/2
2	NAP	B	603	-	-	0/27/67/67	0/5/5/5
5	EDO	B	604	-	-	0/1/1/1	0/0/0/0
5	EDO	B	605	-	-	0/1/1/1	0/0/0/0
5	EDO	B	606	-	-	0/1/1/1	0/0/0/0
5	EDO	B	607	-	-	0/1/1/1	0/0/0/0
5	EDO	B	608	-	-	0/1/1/1	0/0/0/0
5	EDO	B	609	-	-	0/1/1/1	0/0/0/0
5	EDO	B	610	-	-	0/1/1/1	0/0/0/0
5	EDO	B	611	-	-	0/1/1/1	0/0/0/0
5	EDO	B	612	-	-	0/1/1/1	0/0/0/0
5	EDO	B	613	-	-	0/1/1/1	0/0/0/0
5	EDO	B	614	-	-	0/1/1/1	0/0/0/0
5	EDO	B	615	-	-	0/1/1/1	0/0/0/0
3	THG	C	601	-	-	0/16/31/31	0/3/3/3
2	NAP	C	602	-	-	0/27/67/67	0/5/5/5
4	UMP	C	603	-	-	0/6/22/22	0/2/2/2
5	EDO	C	604	-	-	0/1/1/1	0/0/0/0
5	EDO	C	605	-	-	0/1/1/1	0/0/0/0
5	EDO	C	606	-	-	0/1/1/1	0/0/0/0
5	EDO	C	607	-	-	0/1/1/1	0/0/0/0
5	EDO	C	608	-	-	0/1/1/1	0/0/0/0
5	EDO	C	609	-	-	0/1/1/1	0/0/0/0
5	EDO	C	610	-	-	0/1/1/1	0/0/0/0
5	EDO	C	611	-	-	0/1/1/1	0/0/0/0
5	EDO	C	612	-	-	0/1/1/1	0/0/0/0
5	EDO	C	613	-	-	0/1/1/1	0/0/0/0
5	EDO	C	614	-	-	0/1/1/1	0/0/0/0
2	NAP	D	701	-	-	0/27/67/67	0/5/5/5
4	UMP	D	702	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THG	D	703	-	-	0/16/31/31	0/3/3/3
5	EDO	D	704	-	-	0/1/1/1	0/0/0/0
5	EDO	D	705	-	-	0/1/1/1	0/0/0/0
5	EDO	D	706	-	-	0/1/1/1	0/0/0/0
5	EDO	D	707	-	-	0/1/1/1	0/0/0/0
5	EDO	D	708	-	-	0/1/1/1	0/0/0/0
5	EDO	D	709	-	-	0/1/1/1	0/0/0/0
5	EDO	D	710	-	-	0/1/1/1	0/0/0/0
5	EDO	D	711	-	-	0/1/1/1	0/0/0/0
5	EDO	D	712	-	-	0/1/1/1	0/0/0/0
5	EDO	D	713	-	-	0/1/1/1	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	UMP	P-OP2	-2.27	1.45	1.54
2	C	602	NAP	C5A-N7A	-2.22	1.31	1.39
4	B	602	UMP	C6-C5	-2.13	1.33	1.38
3	B	601	THG	C3'-C4'	2.01	1.42	1.39
3	B	601	THG	C2'-C1'	2.01	1.42	1.39

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAP	N3A-C2A-N1A	-9.45	120.63	128.86
2	C	602	NAP	N3A-C2A-N1A	-8.35	121.59	128.86
3	B	601	THG	CB-CA-C	-6.99	102.13	112.28
2	B	603	NAP	N3A-C2A-N1A	-6.83	122.91	128.86
2	D	701	NAP	N3A-C2A-N1A	-6.76	122.97	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAP	5	0
3	A	702	THG	3	0
4	A	703	UMP	4	0
5	A	708	EDO	1	0
5	A	713	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	714	EDO	2	0
5	A	717	EDO	1	0
3	B	601	THG	2	0
4	B	602	UMP	3	0
2	B	603	NAP	11	0
5	B	606	EDO	2	0
5	B	609	EDO	1	0
5	B	611	EDO	1	0
5	B	612	EDO	1	0
5	B	613	EDO	2	0
5	B	614	EDO	1	0
3	C	601	THG	1	0
2	C	602	NAP	3	0
4	C	603	UMP	5	0
5	C	604	EDO	1	0
5	C	607	EDO	1	0
5	C	610	EDO	3	0
5	C	611	EDO	3	0
5	C	614	EDO	2	0
2	D	701	NAP	8	0
4	D	702	UMP	2	0
3	D	703	THG	3	0
5	D	708	EDO	2	0
5	D	710	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	385:MET	C	386:LEU	N	1.14

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	494/521 (94%)	-0.33	6 (1%) 79 77	13, 22, 45, 66	0
1	B	495/521 (95%)	-0.32	7 (1%) 75 72	13, 21, 44, 69	1 (0%)
1	C	487/521 (93%)	-0.39	4 (0%) 86 84	13, 22, 42, 65	0
1	D	489/521 (93%)	-0.30	10 (2%) 65 61	13, 23, 48, 69	0
All	All	1965/2084 (94%)	-0.33	27 (1%) 75 72	13, 22, 45, 69	1 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	LEU	4.7
1	B	400	LEU	4.0
1	B	334	TYR	3.9
1	D	88	PHE	3.8
1	B	343	TYR	3.8

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
5	EDO	C	610	4/4	0.72	0.31	46.45	32,37,46,47	0
5	EDO	C	606	4/4	0.90	0.22	23.30	34,36,38,43	0
5	EDO	D	713	4/4	0.97	0.14	13.76	30,35,36,38	0
5	EDO	B	608	4/4	0.83	0.17	12.47	39,39,41,48	0
5	EDO	C	611	4/4	0.85	0.26	11.69	22,24,26,31	4
5	EDO	D	710	4/4	0.81	0.18	10.65	40,41,45,47	0
5	EDO	D	708	4/4	0.91	0.20	10.34	29,32,35,38	0
5	EDO	C	609	4/4	0.89	0.13	10.03	32,34,39,39	0
5	EDO	C	614	4/4	0.81	0.20	7.29	38,39,49,53	0
5	EDO	A	714	4/4	0.72	0.19	6.98	38,39,49,51	0
5	EDO	B	612	4/4	0.92	0.22	6.58	34,39,40,41	0
5	EDO	D	705	4/4	0.91	0.14	5.74	31,43,43,51	0
4	UMP	C	603	20/20	0.80	0.24	5.41	27,46,54,54	0
4	UMP	A	703	20/20	0.82	0.24	5.25	25,39,48,50	15
5	EDO	C	613	4/4	0.89	0.28	4.69	38,39,40,41	0
5	EDO	B	607	4/4	0.84	0.20	4.69	33,36,48,63	0
5	EDO	B	606	4/4	0.85	0.16	3.92	37,38,39,42	0
5	EDO	C	608	4/4	0.87	0.17	3.66	35,47,49,71	0
5	EDO	B	609	4/4	0.87	0.20	3.56	34,47,48,49	0
5	EDO	B	613	4/4	0.93	0.17	3.08	38,45,48,52	0
3	THG	D	703	32/32	0.78	0.25	3.01	30,46,64,65	0
5	EDO	A	711	4/4	0.90	0.17	2.99	38,39,44,47	0
4	UMP	D	702	20/20	0.79	0.26	2.78	32,48,62,62	0
5	EDO	B	611	4/4	0.89	0.25	2.75	30,39,43,47	0
5	EDO	A	707	4/4	0.94	0.15	2.57	31,32,32,45	0
4	UMP	B	602	20/20	0.90	0.19	2.33	27,42,48,49	0
5	EDO	C	607	4/4	0.85	0.17	2.27	36,38,40,42	0
5	EDO	D	712	4/4	0.94	0.12	2.16	27,32,33,42	0
3	THG	A	702	32/32	0.89	0.16	2.00	24,38,50,55	0
5	EDO	B	604	4/4	0.92	0.14	1.51	33,36,36,37	0
5	EDO	D	706	4/4	0.87	0.18	1.19	39,42,44,45	0
5	EDO	A	709	4/4	0.92	0.13	1.09	30,31,43,55	0
3	THG	C	601	32/32	0.91	0.13	1.07	27,44,53,55	0
5	EDO	A	713	4/4	0.76	0.19	0.97	42,42,42,57	0
5	EDO	A	715	4/4	0.86	0.17	0.96	52,55,57,58	0
5	EDO	A	704	4/4	0.94	0.11	0.75	27,30,30,34	0
3	THG	B	601	32/32	0.92	0.14	0.70	24,36,44,54	0
2	NAP	D	701	48/48	0.96	0.14	0.70	31,37,112,117	0
5	EDO	A	716	4/4	0.93	0.13	0.61	34,40,42,43	0
5	EDO	A	708	4/4	0.95	0.11	0.59	37,41,43,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	B	603	48/48	0.97	0.12	0.45	23,30,95,101	0
5	EDO	C	612	4/4	0.95	0.10	0.39	23,24,25,27	0
5	EDO	D	704	4/4	0.97	0.10	0.35	21,22,23,25	0
5	EDO	C	605	4/4	0.95	0.10	0.33	36,38,43,51	0
2	NAP	A	701	48/48	0.97	0.12	0.27	25,31,88,97	0
5	EDO	B	605	4/4	0.95	0.10	0.26	23,23,24,25	0
5	EDO	A	710	4/4	0.95	0.10	0.08	28,29,36,44	0
5	EDO	C	604	4/4	0.96	0.09	-0.02	21,21,22,22	0
5	EDO	A	712	4/4	0.95	0.10	-0.04	35,43,46,54	0
2	NAP	C	602	48/48	0.97	0.10	-0.04	25,32,101,111	0
5	EDO	D	709	4/4	0.94	0.11	-0.07	24,25,28,29	0
5	EDO	B	615	4/4	0.95	0.09	-0.45	26,26,27,29	0
5	EDO	A	706	4/4	0.97	0.08	-0.60	22,23,23,26	0
5	EDO	A	705	4/4	0.98	0.08	-1.13	20,22,22,23	0
5	EDO	D	707	4/4	0.87	0.16	-	49,49,52,54	0
5	EDO	A	717	4/4	0.92	0.22	-	46,46,47,54	0
5	EDO	D	711	4/4	0.85	0.12	-	49,52,52,62	0
5	EDO	B	614	4/4	0.93	0.09	-	41,42,45,54	0
5	EDO	B	610	4/4	0.84	0.11	-	47,51,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.