



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2016 – 02:25 PM EDT

PDB ID : 5BPK  
Title : Varying binding modes of inhibitors and structural differences in the binding pockets of different gamma-glutamyltranspeptidases  
Authors : Bolz, C.; Bach, N.C.; Meyer, H.; Mueller, G.; Dawidowski, M.; Popowicz, G.; Sieber, S.A.; Skerra, A.; Gerhard, M.  
Deposited on : 2015-05-28  
Resolution : 1.49 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](mailto: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.

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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-20027457  
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-20027457

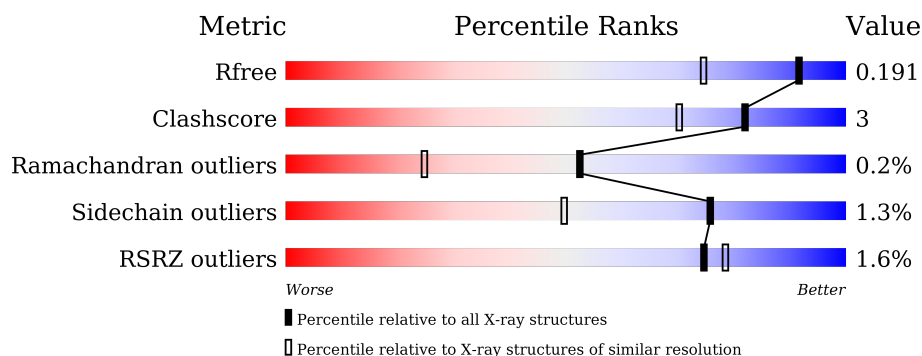
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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  $\geq 3$ , 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	379	<div> <div>88%</div> <div>8%</div> </div>
1	B	379	<div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
2	C	225	<div> <div>76%</div> <div>7%</div> <div>16%</div> </div>
2	D	225	<div> <div>76%</div> <div>8%</div> <div>16%</div> </div>

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	EDO	A	402	-	-	-	X
3	EDO	A	404	-	-	-	X
3	EDO	A	408	-	-	-	X
3	EDO	A	409	-	-	-	X
3	EDO	B	401	-	-	-	X
3	EDO	B	403	-	-	-	X
3	EDO	B	407	-	-	-	X
3	EDO	B	411	-	-	-	X
3	EDO	B	412	-	-	-	X
3	EDO	C	702	-	-	-	X
3	EDO	C	703	-	-	-	X
3	EDO	C	706	-	-	-	X
3	EDO	C	708	-	-	-	X
3	EDO	C	710	-	-	-	X
3	EDO	C	711	-	-	-	X
3	EDO	D	702	-	-	-	X
3	EDO	D	704	-	-	-	X
3	EDO	D	709	-	-	-	X
3	EDO	D	710	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9438 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 Gamma-glutamyltranspeptidase (Ggt).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	22	3	0
			2662	1699	455	498	10			
1	B	348	Total	C	N	O	S	24	10	0
			2713	1731	462	510	10			

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase (Ggt).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	188	Total	C	N	O	S	14	3	0
			1457	922	248	280	7			
2	D	188	Total	C	N	O	S	10	3	0
			1453	921	245	280	7			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	568	GLY	-	expression tag	UNP O25743
C	569	THR	-	expression tag	UNP O25743
C	570	GLY	-	expression tag	UNP O25743
C	571	SER	-	expression tag	UNP O25743
C	572	LYS	-	expression tag	UNP O25743
C	573	LEU	-	expression tag	UNP O25743
C	574	ALA	-	expression tag	UNP O25743
C	575	ALA	-	expression tag	UNP O25743
C	576	ALA	-	expression tag	UNP O25743
C	577	GLN	-	expression tag	UNP O25743
C	578	LEU	-	expression tag	UNP O25743
C	579	TYR	-	expression tag	UNP O25743
C	580	THR	-	expression tag	UNP O25743
C	581	ARG	-	expression tag	UNP O25743
C	582	ALA	-	expression tag	UNP O25743
C	583	SER	-	expression tag	UNP O25743

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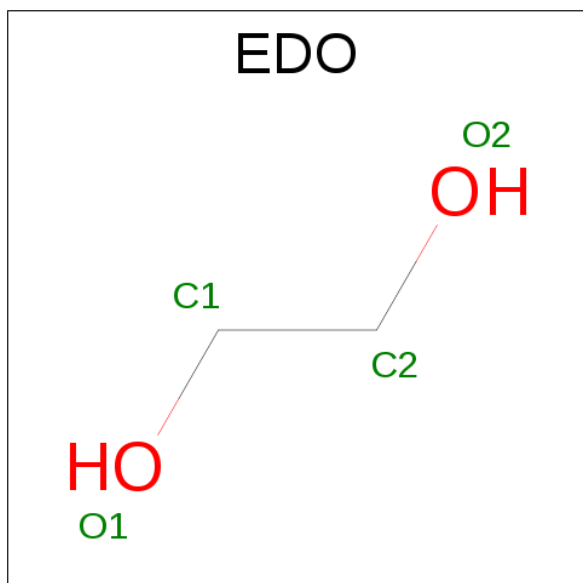
Chain	Residue	Modelled	Actual	Comment	Reference
C	584	GLN	-	expression tag	UNP O25743
C	585	PRO	-	expression tag	UNP O25743
C	586	GLU	-	expression tag	UNP O25743
C	587	LEU	-	expression tag	UNP O25743
C	588	ALA	-	expression tag	UNP O25743
C	589	PRO	-	expression tag	UNP O25743
C	590	GLU	-	expression tag	UNP O25743
C	591	ASP	-	expression tag	UNP O25743
C	592	PRO	-	expression tag	UNP O25743
C	593	GLU	-	expression tag	UNP O25743
C	594	ASP	-	expression tag	UNP O25743
C	595	LEU	-	expression tag	UNP O25743
C	596	GLU	-	expression tag	UNP O25743
C	597	HIS	-	expression tag	UNP O25743
C	598	HIS	-	expression tag	UNP O25743
C	599	HIS	-	expression tag	UNP O25743
C	600	HIS	-	expression tag	UNP O25743
C	601	HIS	-	expression tag	UNP O25743
C	602	HIS	-	expression tag	UNP O25743
C	603	HIS	-	expression tag	UNP O25743
C	604	HIS	-	expression tag	UNP O25743
D	568	GLY	-	expression tag	UNP O25743
D	569	THR	-	expression tag	UNP O25743
D	570	GLY	-	expression tag	UNP O25743
D	571	SER	-	expression tag	UNP O25743
D	572	LYS	-	expression tag	UNP O25743
D	573	LEU	-	expression tag	UNP O25743
D	574	ALA	-	expression tag	UNP O25743
D	575	ALA	-	expression tag	UNP O25743
D	576	ALA	-	expression tag	UNP O25743
D	577	GLN	-	expression tag	UNP O25743
D	578	LEU	-	expression tag	UNP O25743
D	579	TYR	-	expression tag	UNP O25743
D	580	THR	-	expression tag	UNP O25743
D	581	ARG	-	expression tag	UNP O25743
D	582	ALA	-	expression tag	UNP O25743
D	583	SER	-	expression tag	UNP O25743
D	584	GLN	-	expression tag	UNP O25743
D	585	PRO	-	expression tag	UNP O25743
D	586	GLU	-	expression tag	UNP O25743
D	587	LEU	-	expression tag	UNP O25743
D	588	ALA	-	expression tag	UNP O25743

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Chain	Residue	Modelled	Actual	Comment	Reference
D	589	PRO	-	expression tag	UNP O25743
D	590	GLU	-	expression tag	UNP O25743
D	591	ASP	-	expression tag	UNP O25743
D	592	PRO	-	expression tag	UNP O25743
D	593	GLU	-	expression tag	UNP O25743
D	594	ASP	-	expression tag	UNP O25743
D	595	LEU	-	expression tag	UNP O25743
D	596	GLU	-	expression tag	UNP O25743
D	597	HIS	-	expression tag	UNP O25743
D	598	HIS	-	expression tag	UNP O25743
D	599	HIS	-	expression tag	UNP O25743
D	600	HIS	-	expression tag	UNP O25743
D	601	HIS	-	expression tag	UNP O25743
D	602	HIS	-	expression tag	UNP O25743
D	603	HIS	-	expression tag	UNP O25743
D	604	HIS	-	expression tag	UNP O25743

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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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	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	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
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

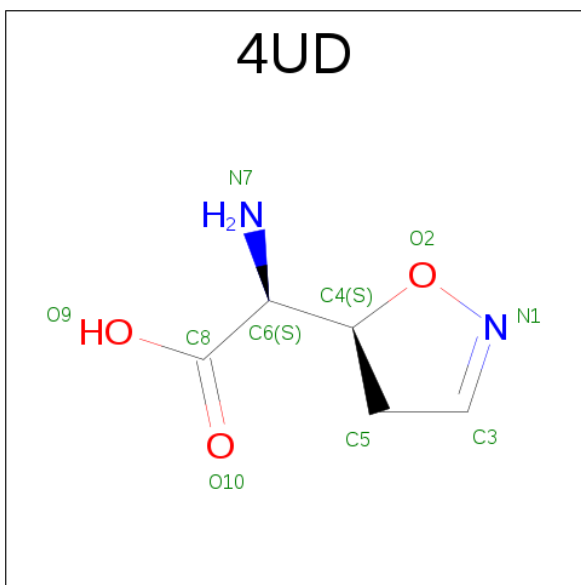
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0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

- Molecule 4 is (2S)-amino[(5S)-4,5-dihydro-1,2-oxazol-5-yl]acetic acid (three-letter code: 4UD) (formula: C<sub>5</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			10	5	2	3		
4	D	1	Total	C	N	O	0	0
			10	5	2	3		

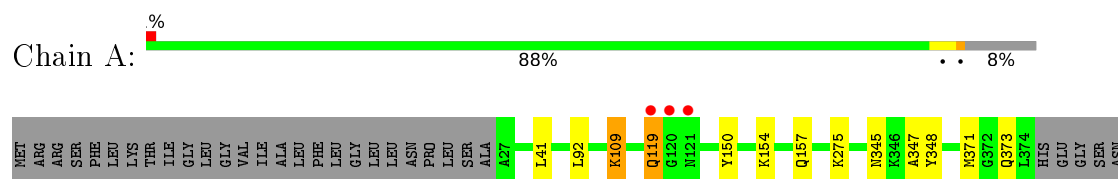
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	333	Total	O	0	0
			333	333		
5	C	148	Total	O	0	1
			149	149		
5	B	331	Total	O	0	0
			331	331		
5	D	146	Total	O	0	2
			148	148		

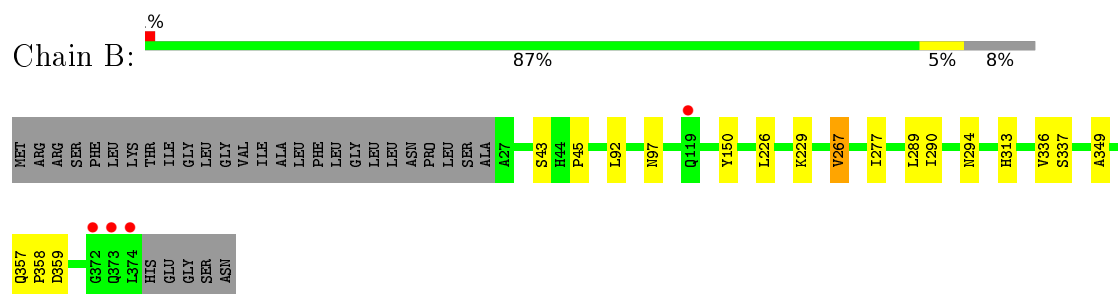
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

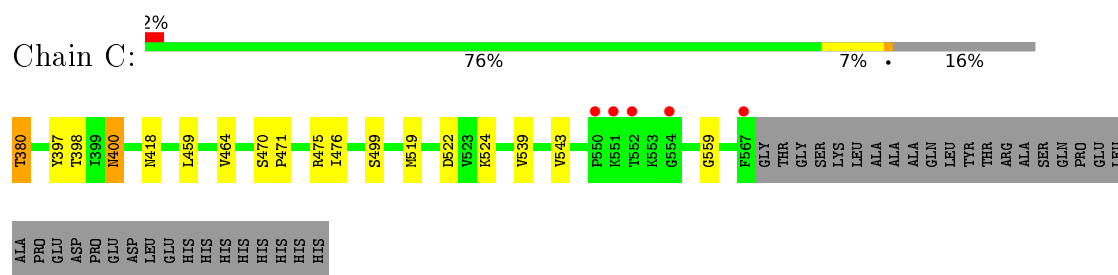
- Molecule 1: Gamma-glutamyltranspeptidase (Ggt)



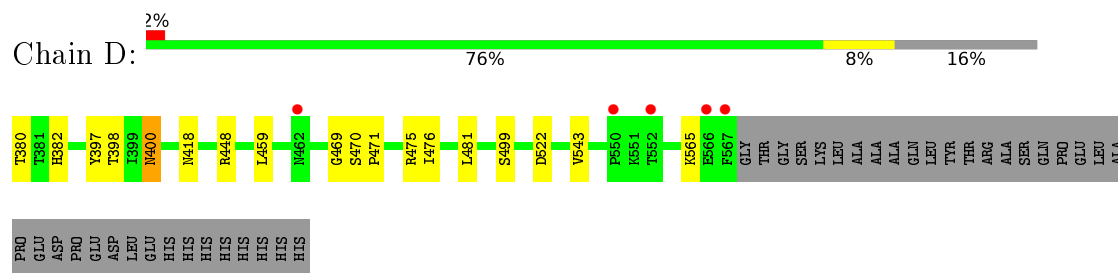
- Molecule 1: Gamma-glutamyltranspeptidase (Ggt)



- Molecule 2: Gamma-glutamyltranspeptidase (Ggt)



- Molecule 2: Gamma-glutamyltranspeptidase (Ggt)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.78Å 112.01Å 91.85Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	91.80 – 1.49 47.82 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.80-1.49) 99.2 (47.82-1.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.49Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.144 , 0.184 0.153 , 0.191	Depositor DCC
$R_{free}$ test set	4718 reflections (2.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 4UD, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/2710	0.57	0/3650
1	B	0.40	0/2762	0.58	0/3724
2	C	0.42	0/1487	0.63	0/2020
2	D	0.44	0/1483	0.65	1/2016 (0.0%)
All	All	0.41	0/8442	0.60	1/11410 (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	448	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2662	0	2728	8	0
1	B	2713	0	2773	17	0
2	C	1457	0	1448	18	0
2	D	1453	0	1444	18	0
3	A	40	0	60	0	0
3	B	52	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	40	0	60	2	0
3	D	40	0	60	1	0
4	C	10	0	0	2	0
4	D	10	0	0	2	0
5	A	333	0	0	2	0
5	B	331	0	0	1	0
5	C	149	0	0	1	0
5	D	148	0	0	2	0
All	All	9438	0	8651	55	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 (55) 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)
2:D:499[A]:SER:OG	5:D:801:HOH:O	1.84	0.95
2:D:380[B]:THR:HB	2:D:471:PRO:HB3	1.58	0.86
2:C:380[A]:THR:HB	2:C:471:PRO:HB3	1.60	0.81
1:B:358[B]:PRO:O	5:B:501:HOH:O	2.05	0.74
2:C:380[A]:THR:HG23	2:C:398:THR:HB	1.72	0.72
2:D:380[B]:THR:HG23	2:D:398:THR:HB	1.74	0.69
2:D:380[B]:THR:HG21	4:D:701:4UD:N1	2.09	0.68
1:B:313:HIS:HE1	1:B:357[B]:GLN:O	1.76	0.67
2:D:380[B]:THR:HB	2:D:471:PRO:CB	2.25	0.67
1:B:277[A]:ILE:HD11	2:D:459:LEU:HD11	1.78	0.66
1:A:92:LEU:HD11	1:A:150:TYR:CE1	2.30	0.65
2:C:380[B]:THR:N	2:C:398:THR:HG1	1.94	0.65
2:D:380[A]:THR:O	2:D:380[A]:THR:HG23	1.96	0.65
2:D:380[A]:THR:N	2:D:398:THR:HG1	1.95	0.64
2:C:380[B]:THR:O	2:C:380[B]:THR:HG23	1.96	0.64
1:A:348:TYR:CE1	1:A:371:MET:HE2	2.34	0.62
2:C:380[A]:THR:HG21	4:C:701:4UD:N1	2.12	0.62
1:B:358[A]:PRO:O	1:B:359[A]:ASP:HB2	2.04	0.58
1:B:43:SER:O	2:D:565:LYS:HD2	2.02	0.58
1:A:109:LYS:HD2	5:A:512:HOH:O	2.04	0.57
1:B:289[B]:LEU:CD2	2:D:481:LEU:HB3	2.35	0.57
2:C:380[A]:THR:HB	2:C:471:PRO:CB	2.33	0.57
1:B:277[A]:ILE:HD11	2:D:459:LEU:CD1	2.35	0.56
1:B:92:LEU:HD11	1:B:150:TYR:CE1	2.42	0.55
2:C:539:VAL:HG13	3:C:709:EDO:H22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[B]:LEU:HD23	2:D:481:LEU:HB3	1.90	0.53
2:C:464:VAL:HG23	3:C:702:EDO:H12	1.89	0.53
1:A:119:GLN:N	1:A:119:GLN:HE21	2.10	0.50
2:D:400:ASN:HB3	2:D:418:ASN:OD1	2.12	0.49
2:C:380[B]:THR:O	2:C:380[B]:THR:CG2	2.61	0.49
2:C:380[A]:THR:HG23	2:C:398:THR:CB	2.42	0.49
2:C:380[A]:THR:CG2	2:C:398:THR:HB	2.42	0.49
1:A:345:ASN:OD1	1:A:347:ALA:HB3	2.14	0.48
1:B:226:LEU:O	1:B:229:LYS:HG2	2.14	0.48
2:D:380[A]:THR:O	2:D:380[A]:THR:CG2	2.62	0.47
2:C:400:ASN:HB3	2:C:418:ASN:OD1	2.16	0.46
2:C:476:ILE:HD11	4:C:701:4UD:N1	2.29	0.46
2:D:470:SER:HB2	2:D:543:VAL:HG22	1.96	0.46
2:D:476:ILE:HD11	4:D:701:4UD:N1	2.31	0.46
1:A:154:LYS:H	1:A:157:GLN:HE21	1.65	0.45
2:C:499[A]:SER:OG	5:C:802:HOH:O	2.20	0.45
1:A:275:LYS:HD2	2:C:459:LEU:HD12	1.99	0.45
2:C:519:MET:SD	2:C:524:LYS:HG2	2.56	0.44
2:D:382:HIS:CE1	2:D:469:GLY:HA3	2.53	0.44
5:A:597:HOH:O	3:D:702:EDO:H12	2.17	0.44
1:B:357[B]:GLN:HE21	1:B:357[B]:GLN:HA	1.84	0.43
1:B:97:ASN:OD1	1:B:277[A]:ILE:HD13	2.19	0.42
1:B:336[B]:VAL:HG21	5:D:933:HOH:O	2.19	0.42
1:A:41:LEU:HD11	2:C:559:GLY:HA3	2.03	0.41
1:B:336[B]:VAL:HG22	1:B:337:SER:N	2.35	0.41
1:B:294:ASN:HB3	1:B:349:ALA:CB	2.52	0.40
2:D:380[B]:THR:HG23	2:D:398:THR:CB	2.47	0.40
1:B:267[B]:VAL:HG13	1:B:290:ILE:HD12	2.03	0.40
1:B:45:PRO:HA	3:B:405:EDO:H11	2.04	0.40
2:C:470:SER:HB2	2:C:543:VAL:HG22	2.03	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	349/379 (92%)	344 (99%)	5 (1%)	0	100	100
1	B	356/379 (94%)	352 (99%)	4 (1%)	0	100	100
2	C	188/225 (84%)	181 (96%)	6 (3%)	1 (0%)	34	10
2	D	188/225 (84%)	182 (97%)	5 (3%)	1 (0%)	34	10
All	All	1081/1208 (90%)	1059 (98%)	20 (2%)	2 (0%)	52	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	400	ASN
2	D	400	ASN

### 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	277/299 (93%)	274 (99%)	3 (1%)	80	58
1	B	284/299 (95%)	282 (99%)	2 (1%)	88	73
2	C	162/189 (86%)	157 (97%)	5 (3%)	47	14
2	D	162/189 (86%)	159 (98%)	3 (2%)	65	31
All	All	885/976 (91%)	872 (98%)	13 (2%)	76	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	119	GLN
1	A	373	GLN
2	C	380[A]	THR
2	C	380[B]	THR
2	C	397	TYR

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Mol	Chain	Res	Type
2	C	475	ARG
2	C	522	ASP
1	B	267[A]	VAL
1	B	267[B]	VAL
2	D	397	TYR
2	D	475	ARG
2	D	522	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	157	GLN
1	A	202	HIS
1	A	366	GLN
1	A	373	GLN
2	C	462	ASN
1	B	168	ASN
1	B	174	GLN
1	B	313	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

45 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	401	-	3,3,3	0.46	0	2,2,2	0.42	0
3	EDO	A	402	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	A	403	-	3,3,3	0.37	0	2,2,2	0.38	0
3	EDO	A	404	-	3,3,3	0.65	0	2,2,2	0.17	0
3	EDO	A	405	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	A	406	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	A	408	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	A	409	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.43	0
3	EDO	B	403	-	3,3,3	0.38	0	2,2,2	0.41	0
3	EDO	B	404	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	B	405	-	3,3,3	0.56	0	2,2,2	0.21	0
3	EDO	B	406	-	3,3,3	0.43	0	2,2,2	0.27	0
3	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	B	408	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	B	409	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	B	410	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	B	411	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	B	412	-	3,3,3	0.41	0	2,2,2	0.48	0
3	EDO	B	413	-	3,3,3	0.34	0	2,2,2	0.52	0
4	4UD	C	701	2	6,10,10	2.61	3 (50%)	2,13,13	4.57	1 (50%)
3	EDO	C	702	-	3,3,3	0.56	0	2,2,2	0.05	0
3	EDO	C	703	-	3,3,3	0.51	0	2,2,2	0.14	0
3	EDO	C	704	-	3,3,3	0.57	0	2,2,2	0.25	0
3	EDO	C	705	-	3,3,3	0.50	0	2,2,2	0.30	0
3	EDO	C	706	-	3,3,3	0.37	0	2,2,2	0.52	0
3	EDO	C	707	-	3,3,3	0.47	0	2,2,2	0.21	0
3	EDO	C	708	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	C	709	-	3,3,3	0.35	0	2,2,2	0.47	0
3	EDO	C	710	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	C	711	-	3,3,3	0.35	0	2,2,2	0.47	0
4	4UD	D	701	2	6,10,10	2.50	3 (50%)	2,13,13	4.21	1 (50%)
3	EDO	D	702	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	D	703	-	3,3,3	0.45	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	704	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	D	705	-	3,3,3	0.56	0	2,2,2	0.22	0
3	EDO	D	706	-	3,3,3	0.50	0	2,2,2	0.56	0
3	EDO	D	707	-	3,3,3	0.34	0	2,2,2	0.36	0
3	EDO	D	708	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	D	709	-	3,3,3	0.45	0	2,2,2	0.30	0
3	EDO	D	710	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	D	711	-	3,3,3	0.44	0	2,2,2	0.37	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	401	-	-	0/1/1/1	0/0/0/0
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
3	EDO	A	404	-	-	0/1/1/1	0/0/0/0
3	EDO	A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	B	401	-	-	0/1/1/1	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	EDO	B	405	-	-	0/1/1/1	0/0/0/0
3	EDO	B	406	-	-	0/1/1/1	0/0/0/0
3	EDO	B	407	-	-	0/1/1/1	0/0/0/0
3	EDO	B	408	-	-	0/1/1/1	0/0/0/0
3	EDO	B	409	-	-	0/1/1/1	0/0/0/0
3	EDO	B	410	-	-	0/1/1/1	0/0/0/0
3	EDO	B	411	-	-	0/1/1/1	0/0/0/0
3	EDO	B	412	-	-	0/1/1/1	0/0/0/0
3	EDO	B	413	-	-	0/1/1/1	0/0/0/0
4	4UD	C	701	2	-	0/3/15/15	0/1/1/1
3	EDO	C	702	-	-	0/1/1/1	0/0/0/0
3	EDO	C	703	-	-	0/1/1/1	0/0/0/0
3	EDO	C	704	-	-	0/1/1/1	0/0/0/0
3	EDO	C	705	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	706	-	-	0/1/1/1	0/0/0/0
3	EDO	C	707	-	-	0/1/1/1	0/0/0/0
3	EDO	C	708	-	-	0/1/1/1	0/0/0/0
3	EDO	C	709	-	-	0/1/1/1	0/0/0/0
3	EDO	C	710	-	-	0/1/1/1	0/0/0/0
3	EDO	C	711	-	-	0/1/1/1	0/0/0/0
4	4UD	D	701	2	-	0/3/15/15	0/1/1/1
3	EDO	D	702	-	-	0/1/1/1	0/0/0/0
3	EDO	D	703	-	-	0/1/1/1	0/0/0/0
3	EDO	D	704	-	-	0/1/1/1	0/0/0/0
3	EDO	D	705	-	-	0/1/1/1	0/0/0/0
3	EDO	D	706	-	-	0/1/1/1	0/0/0/0
3	EDO	D	707	-	-	0/1/1/1	0/0/0/0
3	EDO	D	708	-	-	0/1/1/1	0/0/0/0
3	EDO	D	709	-	-	0/1/1/1	0/0/0/0
3	EDO	D	710	-	-	0/1/1/1	0/0/0/0
3	EDO	D	711	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	4UD	O2-N1	-5.35	1.34	1.42
4	D	701	4UD	O2-N1	-5.09	1.34	1.42
4	D	701	4UD	O2-C4	-2.52	1.43	1.46
4	C	701	4UD	O2-C4	-2.50	1.43	1.46
4	D	701	4UD	C3-N1	2.17	1.29	1.26
4	C	701	4UD	C3-N1	2.27	1.29	1.26

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	4UD	C4-O2-N1	-6.26	102.31	109.00
4	D	701	4UD	C4-O2-N1	-5.91	102.69	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	4UD	2	0
3	C	702	EDO	1	0
3	C	709	EDO	1	0
4	D	701	4UD	2	0
3	D	702	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	348/379 (91%)	-0.18	3 (0%) 85 87	10, 15, 27, 41	8 (2%)
1	B	348/379 (91%)	-0.16	4 (1%) 82 85	8, 15, 26, 49	8 (2%)
2	C	188/225 (83%)	-0.05	5 (2%) 58 61	9, 13, 26, 46	5 (2%)
2	D	188/225 (83%)	-0.05	5 (2%) 58 61	9, 13, 24, 42	3 (1%)
All	All	1072/1208 (88%)	-0.13	17 (1%) 74 78	8, 14, 27, 49	24 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	567	PHE	8.2
1	B	372	GLY	7.2
2	D	567	PHE	5.6
1	B	374	LEU	3.9
1	A	119	GLN	3.7
1	B	373	GLN	3.4
2	C	552	THR	3.2
2	D	552	THR	2.9
1	A	120	GLY	2.7
1	B	119	GLN	2.7
2	D	566	GLU	2.5
2	D	550	PRO	2.5
1	A	121	ASN	2.3
2	D	462	ASN	2.3
2	C	551	LYS	2.2
2	C	554	GLY	2.1
2	C	550	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	C	710	4/4	0.79	0.26	10.79	31,35,37,38	0
3	EDO	C	711	4/4	0.90	0.21	9.09	33,36,38,41	0
3	EDO	D	710	4/4	0.62	0.23	8.82	44,45,46,46	0
3	EDO	B	401	4/4	0.88	0.25	8.78	41,42,44,46	0
3	EDO	D	704	4/4	0.91	0.15	7.88	34,39,39,42	0
3	EDO	A	409	4/4	0.77	0.24	6.48	37,39,41,42	0
3	EDO	C	702	4/4	0.75	0.29	6.37	28,32,32,35	0
3	EDO	A	408	4/4	0.94	0.16	5.75	32,32,32,34	0
3	EDO	D	709	4/4	0.91	0.12	5.47	21,27,32,38	0
3	EDO	D	702	4/4	0.77	0.17	5.42	29,32,32,35	0
3	EDO	B	411	4/4	0.87	0.14	5.29	25,29,33,36	0
3	EDO	A	402	4/4	0.88	0.20	4.59	35,37,37,38	0
3	EDO	C	703	4/4	0.88	0.20	4.55	20,30,30,31	0
3	EDO	A	404	4/4	0.94	0.13	3.72	16,17,20,21	0
3	EDO	B	403	4/4	0.95	0.11	3.41	21,28,29,30	0
3	EDO	B	412	4/4	0.82	0.19	3.22	33,36,37,37	0
3	EDO	C	706	4/4	0.95	0.09	2.21	19,24,24,26	0
3	EDO	B	407	4/4	0.85	0.21	2.06	39,44,44,44	0
3	EDO	C	708	4/4	0.96	0.11	2.05	17,19,20,23	0
3	EDO	B	405	4/4	0.86	0.15	1.93	24,25,30,34	0
3	EDO	D	707	4/4	0.99	0.08	1.91	14,18,18,19	0
3	EDO	B	406	4/4	0.95	0.10	1.79	29,32,34,36	0
3	EDO	B	413	4/4	0.96	0.12	1.76	21,26,27,31	0
3	EDO	C	707	4/4	0.91	0.12	1.59	19,25,28,32	0
3	EDO	A	403	4/4	0.92	0.13	1.50	19,22,22,27	0
3	EDO	D	706	4/4	0.93	0.11	1.37	14,16,16,19	0
3	EDO	C	705	4/4	0.95	0.10	1.06	16,16,17,20	0
3	EDO	B	402	4/4	0.89	0.13	0.82	28,30,36,42	0
4	4UD	C	701	10/10	0.94	0.10	0.73	12,13,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	D	708	4/4	0.94	0.09	0.30	17,28,29,29	0
4	4UD	D	701	10/10	0.94	0.10	0.05	11,13,22,22	0
3	EDO	B	408	4/4	0.86	0.11	-0.03	42,42,43,45	0
3	EDO	C	704	4/4	0.97	0.08	-0.27	12,14,15,19	0
3	EDO	D	705	4/4	0.98	0.06	-1.24	13,13,14,18	0
3	EDO	A	405	4/4	0.81	0.14	-	46,47,47,48	0
3	EDO	A	410	4/4	0.78	0.18	-	41,43,43,45	0
3	EDO	D	711	4/4	0.87	0.15	-	28,37,39,41	0
3	EDO	B	410	4/4	0.74	0.14	-	52,53,53,54	0
3	EDO	A	401	4/4	0.90	0.14	-	37,38,39,40	0
3	EDO	C	709	4/4	0.87	0.27	-	29,33,33,40	0
3	EDO	A	407	4/4	0.73	0.14	-	46,47,48,49	0
3	EDO	D	703	4/4	0.88	0.25	-	39,44,46,49	0
3	EDO	B	409	4/4	0.87	0.12	-	28,31,32,35	0
3	EDO	B	404	4/4	0.86	0.16	-	39,42,43,44	0
3	EDO	A	406	4/4	0.72	0.24	-	45,46,48,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.