



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3II0
Title : Crystal structure of human Glutamate oxaloacetate transaminase 1 (GOT1)
Authors : Ugochukwu, E.; Pilka, E.; Cooper, C.; Bray, J.E.; Yue, W.W.; Muniz, J.; Chaikuad, A.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Kavanagh, K.L.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2009-07-31
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

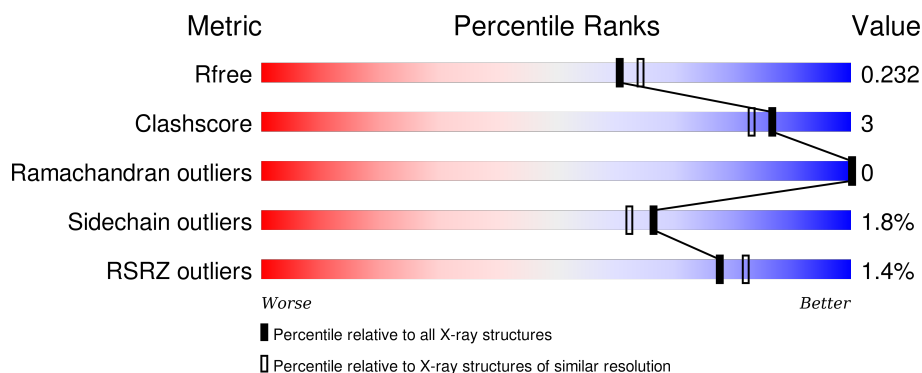
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	422	<div> <div>88%</div> <div>7% . .</div> </div>
1	B	422	<div> <div>90%</div> <div>5% . .</div> </div>
1	C	422	<div> <div>89%</div> <div>8% .</div> </div>
1	D	422	<div> <div>87%</div> <div>9% .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TAR	A	435	X	-	-	-
3	TAR	B	435	X	-	-	-
3	TAR	C	435	X	-	-	-
3	TAR	D	435	X	-	-	-
4	EDO	A	11	-	-	-	X
4	EDO	A	436	-	-	-	X
4	EDO	B	436	-	-	-	X
4	EDO	C	12	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13751 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 Aspartate aminotransferase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	8	7	0
			3222	2063	559	591	9			
1	B	405	Total	C	N	O	S	13	7	0
			3208	2054	556	589	9			
1	C	407	Total	C	N	O	S	0	3	0
			3219	2065	553	591	10			
1	D	407	Total	C	N	O	S	13	2	0
			3213	2058	556	589	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	EXPRESSION TAG	UNP P17174
A	413	ALA	-	EXPRESSION TAG	UNP P17174
A	414	GLU	-	EXPRESSION TAG	UNP P17174
A	415	ASN	-	EXPRESSION TAG	UNP P17174
A	416	LEU	-	EXPRESSION TAG	UNP P17174
A	417	TYR	-	EXPRESSION TAG	UNP P17174
A	418	PHE	-	EXPRESSION TAG	UNP P17174
A	419	GLN	-	EXPRESSION TAG	UNP P17174
A	420	SER	-	EXPRESSION TAG	UNP P17174
A	421	HIS	-	EXPRESSION TAG	UNP P17174
A	422	HIS	-	EXPRESSION TAG	UNP P17174
A	423	HIS	-	EXPRESSION TAG	UNP P17174
A	424	HIS	-	EXPRESSION TAG	UNP P17174
A	425	HIS	-	EXPRESSION TAG	UNP P17174
A	426	HIS	-	EXPRESSION TAG	UNP P17174
A	427	ASP	-	EXPRESSION TAG	UNP P17174
A	428	TYR	-	EXPRESSION TAG	UNP P17174
A	429	LYS	-	EXPRESSION TAG	UNP P17174
A	430	ASP	-	EXPRESSION TAG	UNP P17174
A	431	ASP	-	EXPRESSION TAG	UNP P17174
A	432	ASP	-	EXPRESSION TAG	UNP P17174

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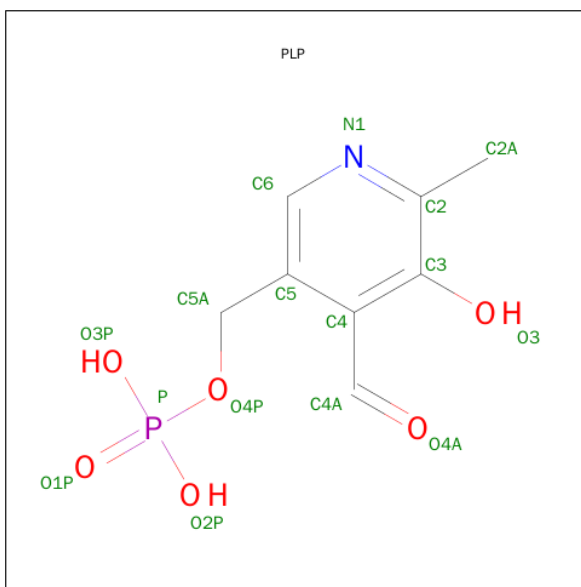
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	ASP	-	EXPRESSION TAG	UNP P17174
A	434	LYS	-	EXPRESSION TAG	UNP P17174
B	13	MET	-	EXPRESSION TAG	UNP P17174
B	413	ALA	-	EXPRESSION TAG	UNP P17174
B	414	GLU	-	EXPRESSION TAG	UNP P17174
B	415	ASN	-	EXPRESSION TAG	UNP P17174
B	416	LEU	-	EXPRESSION TAG	UNP P17174
B	417	TYR	-	EXPRESSION TAG	UNP P17174
B	418	PHE	-	EXPRESSION TAG	UNP P17174
B	419	GLN	-	EXPRESSION TAG	UNP P17174
B	420	SER	-	EXPRESSION TAG	UNP P17174
B	421	HIS	-	EXPRESSION TAG	UNP P17174
B	422	HIS	-	EXPRESSION TAG	UNP P17174
B	423	HIS	-	EXPRESSION TAG	UNP P17174
B	424	HIS	-	EXPRESSION TAG	UNP P17174
B	425	HIS	-	EXPRESSION TAG	UNP P17174
B	426	HIS	-	EXPRESSION TAG	UNP P17174
B	427	ASP	-	EXPRESSION TAG	UNP P17174
B	428	TYR	-	EXPRESSION TAG	UNP P17174
B	429	LYS	-	EXPRESSION TAG	UNP P17174
B	430	ASP	-	EXPRESSION TAG	UNP P17174
B	431	ASP	-	EXPRESSION TAG	UNP P17174
B	432	ASP	-	EXPRESSION TAG	UNP P17174
B	433	ASP	-	EXPRESSION TAG	UNP P17174
B	434	LYS	-	EXPRESSION TAG	UNP P17174
C	13	MET	-	EXPRESSION TAG	UNP P17174
C	413	ALA	-	EXPRESSION TAG	UNP P17174
C	414	GLU	-	EXPRESSION TAG	UNP P17174
C	415	ASN	-	EXPRESSION TAG	UNP P17174
C	416	LEU	-	EXPRESSION TAG	UNP P17174
C	417	TYR	-	EXPRESSION TAG	UNP P17174
C	418	PHE	-	EXPRESSION TAG	UNP P17174
C	419	GLN	-	EXPRESSION TAG	UNP P17174
C	420	SER	-	EXPRESSION TAG	UNP P17174
C	421	HIS	-	EXPRESSION TAG	UNP P17174
C	422	HIS	-	EXPRESSION TAG	UNP P17174
C	423	HIS	-	EXPRESSION TAG	UNP P17174
C	424	HIS	-	EXPRESSION TAG	UNP P17174
C	425	HIS	-	EXPRESSION TAG	UNP P17174
C	426	HIS	-	EXPRESSION TAG	UNP P17174
C	427	ASP	-	EXPRESSION TAG	UNP P17174
C	428	TYR	-	EXPRESSION TAG	UNP P17174

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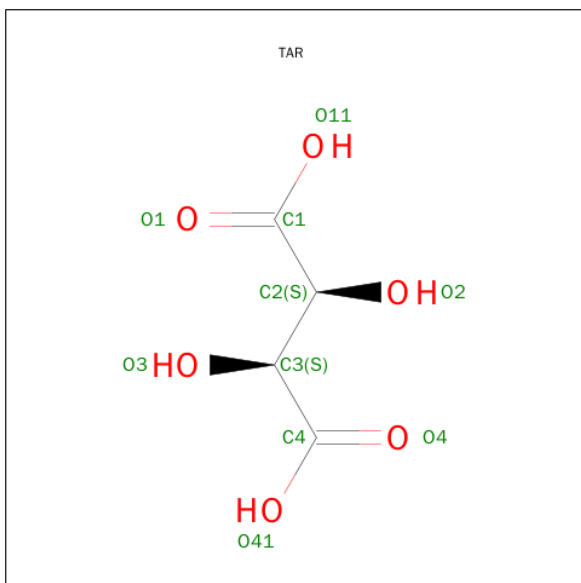
Chain	Residue	Modelled	Actual	Comment	Reference
C	429	LYS	-	EXPRESSION TAG	UNP P17174
C	430	ASP	-	EXPRESSION TAG	UNP P17174
C	431	ASP	-	EXPRESSION TAG	UNP P17174
C	432	ASP	-	EXPRESSION TAG	UNP P17174
C	433	ASP	-	EXPRESSION TAG	UNP P17174
C	434	LYS	-	EXPRESSION TAG	UNP P17174
D	13	MET	-	EXPRESSION TAG	UNP P17174
D	413	ALA	-	EXPRESSION TAG	UNP P17174
D	414	GLU	-	EXPRESSION TAG	UNP P17174
D	415	ASN	-	EXPRESSION TAG	UNP P17174
D	416	LEU	-	EXPRESSION TAG	UNP P17174
D	417	TYR	-	EXPRESSION TAG	UNP P17174
D	418	PHE	-	EXPRESSION TAG	UNP P17174
D	419	GLN	-	EXPRESSION TAG	UNP P17174
D	420	SER	-	EXPRESSION TAG	UNP P17174
D	421	HIS	-	EXPRESSION TAG	UNP P17174
D	422	HIS	-	EXPRESSION TAG	UNP P17174
D	423	HIS	-	EXPRESSION TAG	UNP P17174
D	424	HIS	-	EXPRESSION TAG	UNP P17174
D	425	HIS	-	EXPRESSION TAG	UNP P17174
D	426	HIS	-	EXPRESSION TAG	UNP P17174
D	427	ASP	-	EXPRESSION TAG	UNP P17174
D	428	TYR	-	EXPRESSION TAG	UNP P17174
D	429	LYS	-	EXPRESSION TAG	UNP P17174
D	430	ASP	-	EXPRESSION TAG	UNP P17174
D	431	ASP	-	EXPRESSION TAG	UNP P17174
D	432	ASP	-	EXPRESSION TAG	UNP P17174
D	433	ASP	-	EXPRESSION TAG	UNP P17174
D	434	LYS	-	EXPRESSION TAG	UNP P17174

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



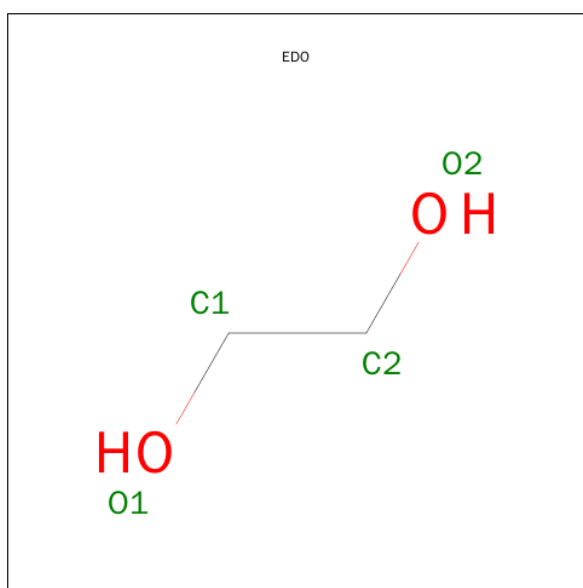
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

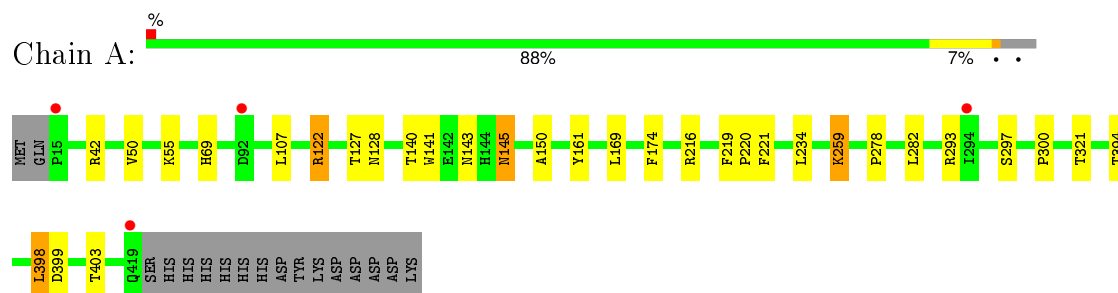
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	218	Total O 218 218	0	0
5	B	205	Total O 205 205	0	0
5	C	162	Total O 162 162	0	0
5	D	148	Total O 148 148	0	0

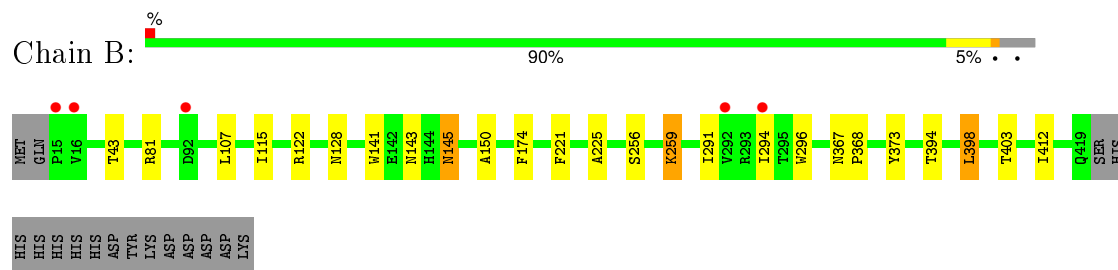
3 Residue-property plots [i](#)

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

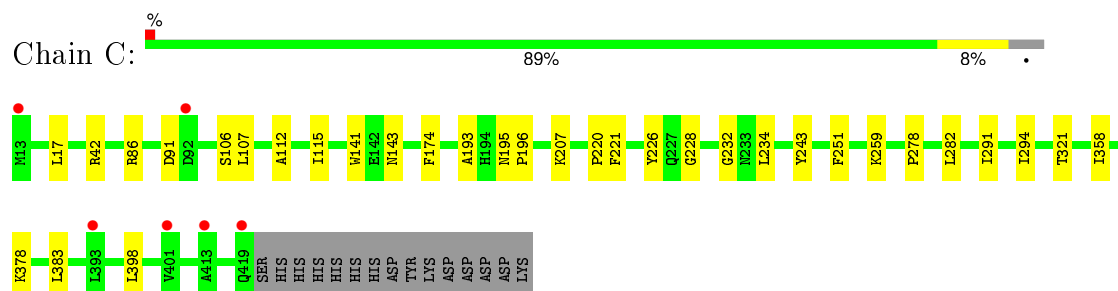
- Molecule 1: Aspartate aminotransferase, cytoplasmic



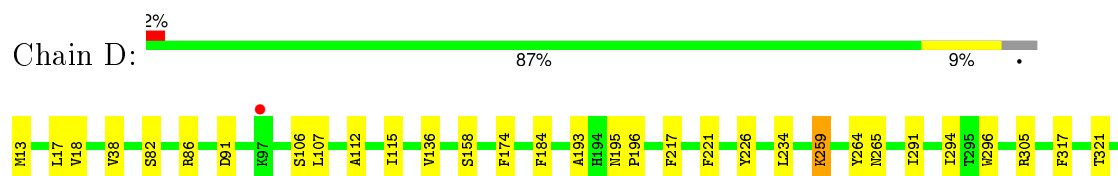
- Molecule 1: Aspartate aminotransferase, cytoplasmic

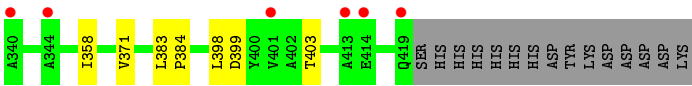


- Molecule 1: Aspartate aminotransferase, cytoplasmic



- Molecule 1: Aspartate aminotransferase, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.53Å 107.35Å 240.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.04 – 2.05 56.04 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.04-2.05) 99.8 (56.04-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.180 , 0.223 0.192 , 0.232	Depositor DCC
R_{free} test set	6410 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 127728 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 38.75 % 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 3.5155e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, TAR, PLP

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	0.71	0/3323	0.75	3/4519 (0.1%)
1	B	0.69	0/3312	0.73	0/4504
1	C	0.69	0/3311	0.71	2/4502 (0.0%)
1	D	0.68	0/3303	0.69	0/4491
All	All	0.69	0/13249	0.72	5/18016 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	42	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	42	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	216	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	42	ARG	NE-CZ-NH1	5.09	122.84	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	3222	0	3135	18	0
1	B	3208	0	3122	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3219	0	3122	17	0
1	D	3213	0	3118	23	0
2	A	16	0	7	1	0
2	B	16	0	7	0	0
2	C	16	0	8	0	0
2	D	16	0	7	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	1	0
4	A	12	0	18	0	0
4	B	12	0	18	4	0
4	C	16	0	24	0	0
4	D	12	0	18	0	0
5	A	218	0	0	1	0
5	B	205	0	0	2	0
5	C	162	0	0	1	0
5	D	148	0	0	0	0
All	All	13751	0	12620	70	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 (70) 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:150:ALA:HB2	1:C:294:ILE:HD12	1.58	0.82
1:D:17:LEU:CD2	1:D:383:LEU:HD22	2.13	0.78
1:C:17:LEU:CD2	1:C:383:LEU:HD22	2.24	0.68
1:C:378:LYS:NZ	5:C:635:HOH:O	2.16	0.64
1:A:259:LYS:NZ	2:A:1:PLP:O4A	2.26	0.63
1:D:17:LEU:HD22	1:D:383:LEU:HD22	1.81	0.63
1:A:150:ALA:HB2	1:D:294:ILE:HD12	1.86	0.56
1:B:373:TYR:HB2	1:B:412:ILE:CD1	2.36	0.56
1:C:358:ILE:C	1:C:358:ILE:HD12	2.29	0.53
1:A:145[A]:ASN:HD22	1:A:145[A]:ASN:C	2.13	0.52
1:A:122[B]:ARG:HD2	1:A:128:ASN:ND2	2.25	0.52
1:D:358:ILE:HD12	1:D:358:ILE:C	2.31	0.51
5:A:578:HOH:O	1:D:305:ARG:NH1	2.44	0.51
1:A:399:ASP:O	1:A:403:THR:HG23	2.11	0.51
1:B:107:LEU:HD11	1:C:107:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD11	1:D:107:LEU:HD11	1.95	0.49
1:C:86:ARG:CD	1:C:91:ASP:OD2	2.61	0.49
1:A:293:ARG:HA	1:A:297:SER:HA	1.95	0.49
1:A:50:VAL:HG11	1:A:55:LYS:HE3	1.94	0.48
1:A:278:PRO:O	1:A:282:LEU:HD23	2.13	0.48
1:A:394:THR:O	1:A:398:LEU:HD22	2.13	0.47
1:C:278:PRO:O	1:C:282:LEU:HD23	2.14	0.47
1:D:18:VAL:HG21	1:D:38:VAL:HA	1.97	0.46
1:B:43:THR:HG22	4:B:1:EDO:H11	1.96	0.46
1:D:86:ARG:CD	1:D:91:ASP:OD2	2.63	0.45
1:B:107:LEU:HD23	1:B:296:TRP:CE2	2.51	0.45
1:A:69:HIS:O	1:D:264:TYR:HB2	2.16	0.45
1:D:107:LEU:HD23	1:D:296:TRP:CE2	2.53	0.45
4:B:436:EDO:H11	5:B:510:HOH:O	2.16	0.45
1:B:394:THR:O	1:B:398:LEU:HD22	2.17	0.45
1:B:141:TRP:CZ3	1:B:143:ASN:HB3	2.52	0.44
1:D:399:ASP:O	1:D:403:THR:HG23	2.18	0.44
1:D:184:PHE:HA	1:D:217:PHE:O	2.16	0.44
1:B:122[A]:ARG:HD2	1:B:128:ASN:ND2	2.33	0.44
1:D:17:LEU:HD21	1:D:383:LEU:HD22	1.98	0.44
1:B:225:ALA:HA	1:B:256:SER:HB3	2.00	0.44
1:B:367:ASN:HB2	1:B:368:PRO:CD	2.47	0.44
1:D:371:VAL:HG11	1:D:384:PRO:HA	1.99	0.44
1:D:106:SER:OG	1:D:112:ALA:HB2	2.18	0.44
1:D:136:VAL:O	1:D:158:SER:HA	2.18	0.44
1:B:259:LYS:N	1:B:259:LYS:HD2	2.33	0.43
1:D:259:LYS:NZ	3:D:435:TAR:O3	2.51	0.43
1:A:140:THR:HG23	1:A:141:TRP:O	2.19	0.43
1:C:141:TRP:CZ3	1:C:143:ASN:HB3	2.54	0.43
1:C:106:SER:OG	1:C:112:ALA:HB2	2.19	0.42
1:D:115:ILE:HD12	1:D:291:ILE:HG22	2.02	0.42
1:C:115:ILE:HD12	1:C:291:ILE:HG22	2.02	0.42
1:C:220:PRO:O	1:C:251:PHE:HB2	2.19	0.42
1:B:81:ARG:CB	4:B:436:EDO:H21	2.49	0.42
1:B:115:ILE:HD12	1:B:291:ILE:HG22	2.01	0.42
1:D:195:ASN:HA	1:D:196:PRO:HA	1.89	0.42
1:C:234:LEU:CD1	1:C:321:THR:HG22	2.50	0.42
4:B:436:EDO:H12	5:B:696:HOH:O	2.19	0.42
1:C:207:LYS:HG2	1:C:243:TYR:CZ	2.55	0.42
1:D:358:ILE:HD12	1:D:358:ILE:O	2.20	0.41
1:C:195:ASN:HA	1:C:196:PRO:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLY:O	1:C:232:GLY:HA2	2.20	0.41
1:A:234:LEU:HD12	1:A:321:THR:HG22	2.02	0.41
1:A:161:TYR:CD1	1:A:169:LEU:HD11	2.55	0.41
1:D:193:ALA:HB3	1:D:226:TYR:HB2	2.02	0.41
1:A:259:LYS:N	1:A:259:LYS:HD2	2.36	0.41
1:A:141:TRP:CZ3	1:A:143:ASN:HB3	2.55	0.41
1:C:193:ALA:HB3	1:C:226:TYR:HB2	2.02	0.41
1:A:300:PRO:HA	1:D:265:ASN:O	2.21	0.41
1:B:122[A]:ARG:CD	1:B:128:ASN:HD21	2.34	0.41
1:D:317:PHE:O	1:D:321:THR:HG23	2.21	0.41
1:C:86:ARG:HD3	1:C:91:ASP:OD2	2.21	0.40
1:A:219:PHE:HA	1:A:220:PRO:HD3	1.96	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	410/422 (97%)	400 (98%)	10 (2%)	0	100	100
1	B	410/422 (97%)	401 (98%)	9 (2%)	0	100	100
1	C	408/422 (97%)	398 (98%)	10 (2%)	0	100	100
1	D	407/422 (96%)	398 (98%)	9 (2%)	0	100	100
All	All	1635/1688 (97%)	1597 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	339/362 (94%)	330 (97%)	9 (3%)	52	45
1	B	337/362 (93%)	330 (98%)	7 (2%)	61	56
1	C	335/362 (92%)	331 (99%)	4 (1%)	78	76
1	D	336/362 (93%)	329 (98%)	7 (2%)	61	56
All	All	1347/1448 (93%)	1320 (98%)	27 (2%)	66	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122[A]	ARG
1	A	122[B]	ARG
1	A	127	THR
1	A	145[A]	ASN
1	A	145[B]	ASN
1	A	174	PHE
1	A	221	PHE
1	A	259	LYS
1	A	398	LEU
1	B	145[A]	ASN
1	B	145[B]	ASN
1	B	174	PHE
1	B	221	PHE
1	B	259	LYS
1	B	294	ILE
1	B	398	LEU
1	C	174	PHE
1	C	221	PHE
1	C	259	LYS
1	C	398	LEU
1	D	13	MET
1	D	82	SER
1	D	174	PHE
1	D	221	PHE
1	D	234	LEU
1	D	259	LYS
1	D	398	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	376	ASN
1	A	406	HIS
1	B	128	ASN
1	B	406	HIS
1	C	176	ASN
1	D	14	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 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	PLP	A	1	-	16,16,16	1.53	2 (12%)	21,23,23	1.58	5 (23%)
4	EDO	A	11	-	3,3,3	0.69	0	2,2,2	0.68	0
4	EDO	A	3	-	3,3,3	0.58	0	2,2,2	0.76	0
3	TAR	A	435	-	3,9,9	0.45	0	6,12,12	1.41	0
4	EDO	A	436	-	3,3,3	0.88	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1	-	3,3,3	0.37	0	2,2,2	0.66	0
4	EDO	B	10	-	3,3,3	0.55	0	2,2,2	0.49	0
2	PLP	B	2	-	16,16,16	1.37	2 (12%)	21,23,23	1.97	5 (23%)
3	TAR	B	435	-	3,9,9	0.92	0	6,12,12	1.11	1 (16%)
4	EDO	B	436	-	3,3,3	0.87	0	2,2,2	0.69	0
4	EDO	C	12	-	3,3,3	0.54	0	2,2,2	0.22	0
2	PLP	C	3	-	16,16,16	1.31	2 (12%)	21,23,23	2.67	7 (33%)
3	TAR	C	435	-	3,9,9	0.45	0	6,12,12	1.10	1 (16%)
4	EDO	C	436	-	3,3,3	0.75	0	2,2,2	0.27	0
4	EDO	C	5	-	3,3,3	0.55	0	2,2,2	1.08	0
4	EDO	C	7	-	3,3,3	0.61	0	2,2,2	0.20	0
2	PLP	D	4	-	16,16,16	1.09	0	21,23,23	2.15	7 (33%)
3	TAR	D	435	-	3,9,9	0.69	0	6,12,12	0.90	0
4	EDO	D	6	-	3,3,3	0.64	0	2,2,2	0.32	0
4	EDO	D	8	-	3,3,3	0.62	0	2,2,2	0.19	0
4	EDO	D	9	-	3,3,3	0.57	0	2,2,2	0.30	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	PLP	A	1	-	-	0/8/8/8	0/1/1/1
4	EDO	A	11	-	-	0/1/1/1	0/0/0/0
4	EDO	A	3	-	-	0/1/1/1	0/0/0/0
3	TAR	A	435	-	2/2/4/4	0/4/12/12	0/0/0/0
4	EDO	A	436	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1	-	-	0/1/1/1	0/0/0/0
4	EDO	B	10	-	-	0/1/1/1	0/0/0/0
2	PLP	B	2	-	-	0/8/8/8	0/1/1/1
3	TAR	B	435	-	2/2/4/4	0/4/12/12	0/0/0/0
4	EDO	B	436	-	-	0/1/1/1	0/0/0/0
4	EDO	C	12	-	-	0/1/1/1	0/0/0/0
2	PLP	C	3	-	-	0/8/8/8	0/1/1/1
3	TAR	C	435	-	2/2/4/4	0/4/12/12	0/0/0/0
4	EDO	C	436	-	-	0/1/1/1	0/0/0/0
4	EDO	C	5	-	-	0/1/1/1	0/0/0/0
4	EDO	C	7	-	-	0/1/1/1	0/0/0/0
2	PLP	D	4	-	-	0/8/8/8	0/1/1/1
3	TAR	D	435	-	2/2/4/4	0/4/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	6	-	-	0/1/1/1	0/0/0/0
4	EDO	D	8	-	-	0/1/1/1	0/0/0/0
4	EDO	D	9	-	-	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)
2	A	1	PLP	C3-C2	-3.99	1.38	1.40
2	C	3	PLP	C3-C2	-3.58	1.38	1.40
2	B	2	PLP	C4-C5	-3.47	1.37	1.42
2	B	2	PLP	C4-C4A	2.15	1.51	1.46
2	A	1	PLP	C4-C4A	2.23	1.51	1.46
2	C	3	PLP	C2-N1	2.42	1.39	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	PLP	C3-C4-C4A	-5.86	110.98	119.84
2	C	3	PLP	O4A-C4A-C4	-3.70	117.64	125.11
2	D	4	PLP	O4A-C4A-C4	-3.17	118.71	125.11
2	C	3	PLP	C5-C4-C4A	-2.95	115.59	122.35
2	C	3	PLP	C5-C6-N1	-2.42	119.66	123.86
2	B	2	PLP	O4A-C4A-C4	-2.41	120.23	125.11
3	B	435	TAR	O3-C3-C4	-2.25	105.54	111.21
2	D	4	PLP	C5-C6-N1	-2.19	120.07	123.86
3	C	435	TAR	O2-C2-C1	-2.17	105.74	111.21
2	A	1	PLP	C5A-C5-C6	-2.10	115.31	119.28
2	D	4	PLP	C3-C4-C5	2.03	119.63	118.11
2	A	1	PLP	O2P-P-O4P	2.11	112.64	106.56
2	C	3	PLP	O3P-P-O2P	2.16	115.62	107.38
2	B	2	PLP	O3-C3-C2	2.20	121.49	117.66
2	A	1	PLP	C5A-C5-C4	2.30	125.33	121.47
2	D	4	PLP	O3-C3-C2	2.49	121.98	117.66
2	B	2	PLP	O4P-P-O1P	2.56	113.67	107.14
2	D	4	PLP	C2A-C2-C3	2.65	124.23	121.04
2	B	2	PLP	C2A-C2-C3	2.82	124.44	121.04
2	A	1	PLP	O3P-P-O4P	3.05	115.35	106.56
2	D	4	PLP	O2P-P-O4P	3.18	115.71	106.56
2	C	3	PLP	O2P-P-O4P	3.65	117.08	106.56
2	A	1	PLP	O4P-C5A-C5	4.07	115.73	108.99
2	D	4	PLP	O4P-C5A-C5	5.82	118.61	108.99
2	B	2	PLP	O4P-C5A-C5	6.54	119.80	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	PLP	O4P-C5A-C5	7.20	120.89	108.99

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	435	TAR	C2
3	C	435	TAR	C3
3	A	435	TAR	C2
3	A	435	TAR	C3
3	D	435	TAR	C2
3	D	435	TAR	C3
3	B	435	TAR	C2
3	B	435	TAR	C3

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PLP	1	0
4	B	1	EDO	1	0
4	B	436	EDO	3	0
3	D	435	TAR	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	405/422 (95%)	-0.32	4 (0%) 84 87	13, 19, 29, 36	2 (0%)
1	B	405/422 (95%)	-0.29	5 (1%) 81 84	13, 19, 28, 35	2 (0%)
1	C	407/422 (96%)	-0.16	6 (1%) 76 81	13, 20, 28, 36	0
1	D	407/422 (96%)	-0.12	7 (1%) 73 78	13, 20, 27, 36	0
All	All	1624/1688 (96%)	-0.22	22 (1%) 78 82	13, 20, 28, 36	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	ALA	5.5
1	C	413	ALA	4.6
1	D	401	VAL	3.7
1	A	15	PRO	3.5
1	C	419	GLN	3.5
1	D	419	GLN	3.3
1	A	419	GLN	3.2
1	D	414	GLU	3.0
1	D	97	LYS	2.8
1	B	15	PRO	2.6
1	A	294	ILE	2.4
1	C	92	ASP	2.4
1	B	16	VAL	2.2
1	D	340	ALA	2.2
1	C	401	VAL	2.1
1	C	393	LEU	2.1
1	D	344	ALA	2.1
1	B	92	ASP	2.1
1	B	294	ILE	2.0
1	B	292	VAL	2.0
1	A	92	ASP	2.0
1	C	13	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	B	436	4/4	0.71	0.23	10.92	38,40,41,43	0
4	EDO	A	11	4/4	0.86	0.21	6.64	27,37,37,38	0
4	EDO	A	436	4/4	0.79	0.19	5.68	42,44,46,48	0
4	EDO	C	12	4/4	0.90	0.15	2.51	41,41,42,44	0
4	EDO	D	8	4/4	0.88	0.16	1.74	36,38,38,42	0
4	EDO	C	436	4/4	0.79	0.13	1.58	31,36,38,38	0
4	EDO	C	5	4/4	0.84	0.16	1.08	28,36,39,43	0
4	EDO	D	9	4/4	0.90	0.10	0.30	43,44,44,44	0
2	PLP	B	2	16/16	0.99	0.12	-0.00	17,22,30,36	0
2	PLP	D	4	16/16	0.99	0.12	-0.12	21,28,33,36	0
2	PLP	A	1	16/16	0.99	0.12	-0.25	20,23,28,31	0
3	TAR	C	435	10/10	0.98	0.11	-0.31	25,27,30,30	0
2	PLP	C	3	16/16	0.99	0.12	-0.32	16,24,37,47	0
3	TAR	B	435	10/10	0.96	0.08	-0.86	20,24,27,28	0
3	TAR	D	435	10/10	0.97	0.08	-1.15	26,28,31,32	0
3	TAR	A	435	10/10	0.97	0.07	-1.86	23,28,30,30	0
4	EDO	A	3	4/4	0.83	0.20	-	37,41,42,44	0
4	EDO	B	1	4/4	0.96	0.14	-	35,35,37,37	0
4	EDO	D	6	4/4	0.81	0.17	-	35,43,47,48	0
4	EDO	B	10	4/4	0.96	0.12	-	34,35,38,39	0
4	EDO	C	7	4/4	0.89	0.14	-	32,40,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.