



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 05:40 PM EDT

PDB ID : 3FTN  
Title : Q165E/S254K Double Mutant Chimera of alcohol dehydrogenase by exchange of the cofactor binding domain res 153-295 of T. brockii ADH by C. beijerinckii ADH  
Authors : Frolov, F.; Gohberg, E.; Shimon, L.; Burstein, Y.  
Deposited on : unknown  
Resolution : 2.19 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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-20030345

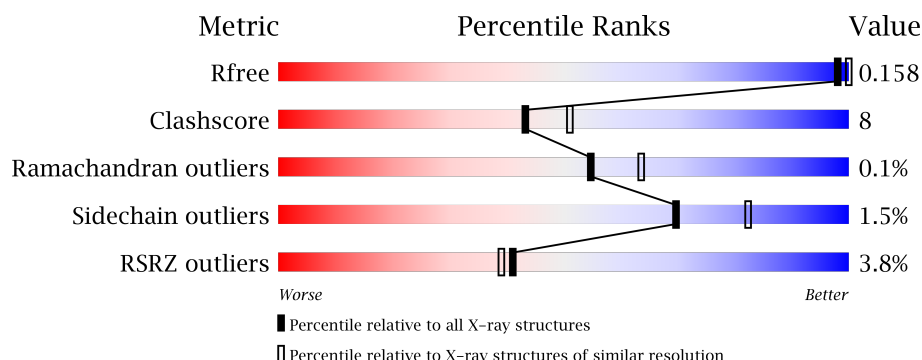
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	352	<div> <div>3%</div> <div>84%</div> <div>16%</div> </div>
1	B	352	<div> <div>2%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	352	<div> <div>2%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	D	352	<div> <div>9%</div> <div>82%</div> <div>16%</div> <div>.</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	ACT	A	353	-	-	-	X
3	ACT	C	355	-	-	-	X
4	EDO	A	355	-	-	-	X
4	EDO	A	356	-	-	-	X
4	EDO	A	358	-	-	-	X
4	EDO	A	360	-	-	-	X
4	EDO	B	358[A]	-	-	-	X
4	EDO	B	358[B]	-	-	-	X
4	EDO	C	356	-	-	-	X
4	EDO	C	359	-	-	-	X
4	EDO	C	360	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11587 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 NADP-dependent alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2651	1693	464	473	21			
1	B	352	Total	C	N	O	S	0	0	0
			2651	1693	464	473	21			
1	C	352	Total	C	N	O	S	0	0	0
			2651	1693	464	473	21			
1	D	352	Total	C	N	O	S	0	0	0
			2651	1693	464	473	21			

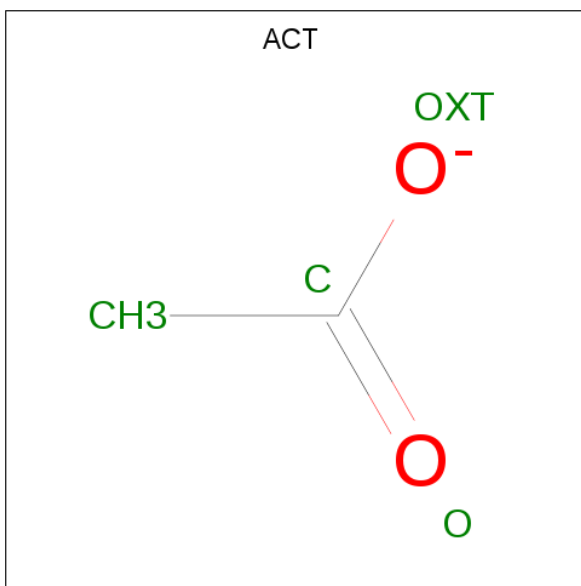
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLU	GLN	ENGINEERED	UNP P25984
A	254	LYS	SER	ENGINEERED	UNP P25984
B	165	GLU	GLN	ENGINEERED	UNP P25984
B	254	LYS	SER	ENGINEERED	UNP P25984
C	165	GLU	GLN	ENGINEERED	UNP P25984
C	254	LYS	SER	ENGINEERED	UNP P25984
D	165	GLU	GLN	ENGINEERED	UNP P25984
D	254	LYS	SER	ENGINEERED	UNP P25984

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

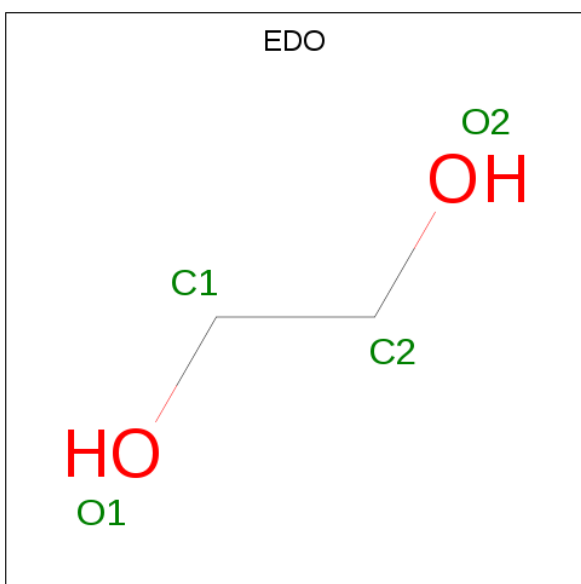
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Cl 3 3	0	0
5	A	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	241	Total O 241 241	0	0
6	B	232	Total O 232 232	0	0
6	C	238	Total O 238 238	0	0

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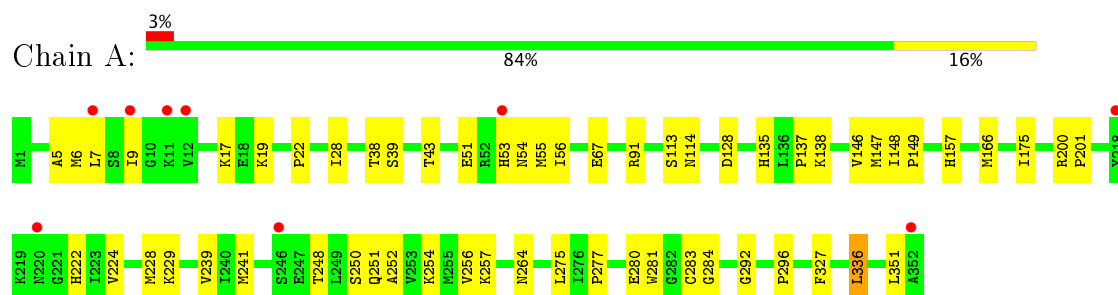
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	194	Total 194	O 194	0	0

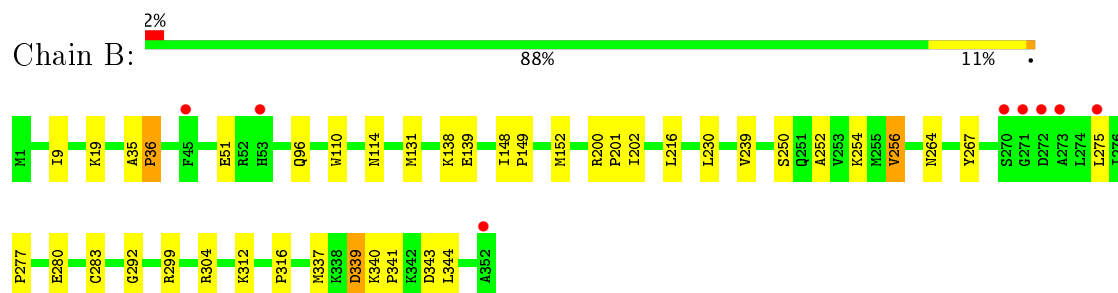
### 3 Residue-property plots [i](#)

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.

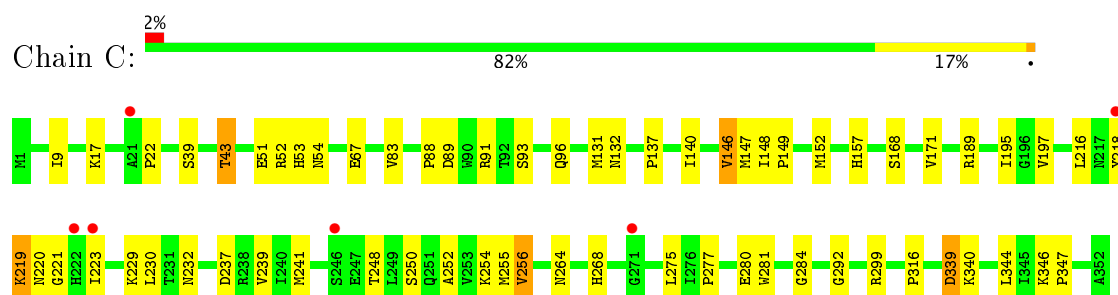
- Molecule 1: NADP-dependent alcohol dehydrogenase



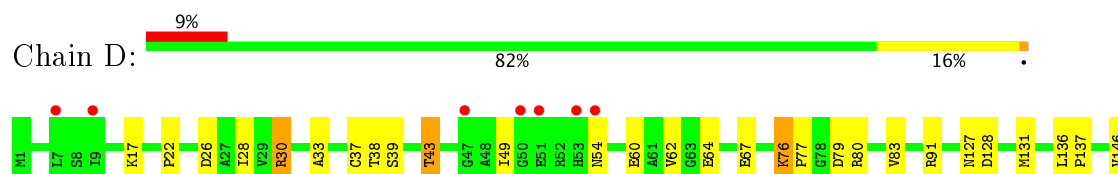
- Molecule 1: NADP-dependent alcohol dehydrogenase



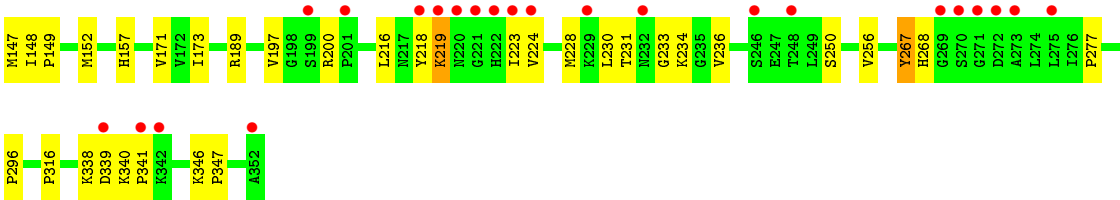
- Molecule 1: NADP-dependent alcohol dehydrogenase



- Molecule 1: NADP-dependent alcohol dehydrogenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.38 Å 83.00 Å 119.69 Å 90.00° 99.93° 90.00°	Depositor
Resolution (Å)	39.18 – 2.19 39.18 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.18-2.19) 97.4 (39.18-2.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.20 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.165 , 0.228 0.159 , 0.158	Depositor DCC
$R_{free}$ test set	3843 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.333 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: ZN, CL, 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	0.42	0/2707	0.58	0/3650
1	B	0.40	0/2707	0.55	0/3650
1	C	0.41	0/2707	0.57	0/3650
1	D	0.38	0/2707	0.53	0/3650
All	All	0.41	0/10828	0.56	0/14600

There are no bond length outliers.

There are no bond angle outliers.

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	2651	0	2707	42	0
1	B	2651	0	2707	35	0
1	C	2651	0	2707	53	0
1	D	2651	0	2707	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	3	0	0
3	C	8	0	6	0	0
4	A	20	0	30	2	0
4	B	12	0	18	3	0
4	C	20	0	30	3	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	241	0	0	12	0
6	B	232	0	0	2	0
6	C	238	0	0	8	0
6	D	194	0	0	6	0
All	All	11587	0	10918	167	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 8.

All (167) 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:220:ASN:HB2	6:C:506:HOH:O	1.63	0.99
1:B:239:VAL:HG23	1:B:256:VAL:HG13	1.43	0.98
1:C:171:VAL:HG11	1:C:255:MET:HE1	1.51	0.91
1:C:239:VAL:HG23	1:C:256:VAL:HG13	1.56	0.85
1:A:239:VAL:HG23	1:A:256:VAL:HG12	1.59	0.82
1:D:22:PRO:HG3	1:D:28:ILE:HG12	1.64	0.79
1:D:76:LYS:HD2	1:D:79:ASP:OD2	1.83	0.78
4:B:358[B]:EDO:H22	1:C:93:SER:HB3	1.67	0.76
1:D:76:LYS:HD3	6:D:724:HOH:O	1.85	0.75
1:A:6:MET:SD	6:A:603:HOH:O	2.44	0.75
1:B:9:ILE:HG13	1:B:51:GLU:HG3	1.70	0.74
1:D:218:TYR:O	1:D:219:LYS:HB3	1.87	0.73
1:A:239:VAL:HG23	1:A:256:VAL:CG1	2.18	0.73
1:A:254:LYS:HG2	1:A:280:GLU:HG2	1.69	0.73
1:D:216:LEU:HD21	1:D:230:LEU:HD11	1.71	0.72
6:A:452:HOH:O	1:D:131:MET:SD	2.48	0.72
1:D:340:LYS:HE2	6:D:748:HOH:O	1.89	0.72
1:A:38:THR:HG22	6:A:457:HOH:O	1.92	0.69
1:C:299:ARG:HD3	4:C:356:EDO:H22	1.76	0.68
1:A:19:LYS:HE2	6:A:528:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:MET:CE	1:C:91:ARG:HB3	2.26	0.66
1:D:38:THR:HG22	6:D:748:HOH:O	1.96	0.65
1:C:229:LYS:HD2	6:C:470:HOH:O	1.97	0.65
1:C:197:VAL:HG11	1:C:223:ILE:HD13	1.77	0.65
1:C:340:LYS:HG3	1:C:344:LEU:HD23	1.78	0.65
1:B:36:PRO:HB2	1:B:337:MET:HG3	1.79	0.65
1:B:131:MET:HG3	1:C:96:GLN:HE21	1.63	0.63
1:A:55:MET:HE1	1:A:114:ASN:N	2.15	0.61
1:A:43:THR:HG21	6:A:654:HOH:O	2.01	0.60
1:C:152:MET:HE1	1:C:316:PRO:HG3	1.84	0.60
1:D:250:SER:OG	1:D:277:PRO:HG3	2.02	0.59
1:D:200:ARG:HG3	6:D:749:HOH:O	2.02	0.59
1:B:131:MET:HG3	1:C:96:GLN:NE2	2.17	0.58
1:C:157:HIS:HE1	4:C:360:EDO:H12	1.67	0.58
1:B:250:SER:OG	1:B:277:PRO:HG3	2.04	0.58
1:B:267:TYR:HE2	6:B:656:HOH:O	1.85	0.58
1:C:219:LYS:C	1:C:221:GLY:H	2.07	0.58
1:B:283:CYS:SG	6:D:508:HOH:O	2.58	0.57
1:D:218:TYR:O	1:D:219:LYS:CB	2.53	0.57
1:A:275:LEU:HD22	1:C:275:LEU:HD22	1.87	0.56
1:C:281:TRP:CE3	1:C:284:GLY:HA2	2.41	0.56
1:A:224:VAL:O	1:A:228:MET:HG2	2.05	0.56
1:B:138:LYS:HE3	1:B:139:GLU:OE2	2.06	0.56
1:B:239:VAL:HG23	1:B:256:VAL:CG1	2.28	0.56
1:D:76:LYS:HD2	1:D:76:LYS:H	1.70	0.56
1:C:83:VAL:O	1:C:149:PRO:HB3	2.06	0.56
1:C:53:HIS:HE1	6:C:541:HOH:O	1.90	0.56
1:A:55:MET:HE1	1:A:113:SER:C	2.27	0.55
1:D:152:MET:HE1	1:D:316:PRO:HG3	1.88	0.55
1:C:250:SER:OG	1:C:277:PRO:HG3	2.07	0.55
1:A:22:PRO:HG3	1:A:28:ILE:HG12	1.89	0.55
1:D:173:ILE:HA	1:D:197:VAL:HB	1.89	0.55
1:A:128:ASP:OD1	1:D:91:ARG:NH1	2.40	0.55
1:A:9:ILE:HG13	1:A:51:GLU:OE2	2.07	0.55
1:C:89:ASP:HB3	6:C:545:HOH:O	2.07	0.55
1:A:250:SER:OG	1:A:277:PRO:HG3	2.06	0.55
4:A:356:EDO:H22	6:A:394:HOH:O	2.06	0.55
1:C:157:HIS:CE1	4:C:360:EDO:H12	2.41	0.54
1:D:76:LYS:HB2	1:D:77:PRO:HD2	1.89	0.54
1:A:175:ILE:HG13	4:A:355:EDO:H21	1.90	0.54
1:A:283:CYS:HB3	1:C:268:HIS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HD2	1:D:128:ASP:OD2	2.09	0.53
1:D:231:THR:O	1:D:234:LYS:HB2	2.08	0.52
1:A:275:LEU:HD22	1:C:275:LEU:CD2	2.40	0.52
1:C:264:ASN:O	1:C:292:GLY:HA2	2.10	0.52
1:C:171:VAL:CG1	1:C:255:MET:HE1	2.34	0.52
1:A:229:LYS:HD3	6:A:450:HOH:O	2.09	0.51
1:D:148:ILE:HB	1:D:149:PRO:HD3	1.91	0.51
1:B:239:VAL:CG2	1:B:256:VAL:HG13	2.27	0.51
1:C:216:LEU:HD21	1:C:230:LEU:HD11	1.92	0.51
1:A:39:SER:O	1:A:43:THR:HG23	2.10	0.51
1:C:39:SER:O	1:C:43:THR:HG23	2.11	0.50
1:B:152:MET:HE1	1:B:316:PRO:HG3	1.93	0.50
1:A:252:ALA:O	1:A:256:VAL:HG13	2.10	0.50
1:B:252:ALA:O	1:B:256:VAL:HG22	2.12	0.50
1:D:37:CYS:HB2	1:D:60:GLU:OE2	2.11	0.50
1:B:131:MET:HE1	1:C:91:ARG:HB3	1.94	0.50
1:B:216:LEU:HD21	1:B:230:LEU:HD11	1.92	0.50
1:B:96:GLN:HE21	1:C:131:MET:CE	2.26	0.48
1:A:166:MET:O	1:B:304:ARG:HG2	2.12	0.48
1:B:202:ILE:HD13	1:B:343:ASP:O	2.13	0.48
1:D:76:LYS:HD2	1:D:76:LYS:N	2.27	0.48
1:C:252:ALA:O	1:C:256:VAL:HG22	2.13	0.48
1:C:171:VAL:HG22	1:C:195:ILE:HB	1.96	0.48
1:C:152:MET:CE	1:C:316:PRO:HG3	2.41	0.48
1:A:146:VAL:HG13	1:A:147:MET:HE2	1.96	0.48
1:A:138:LYS:HE2	6:A:530:HOH:O	2.12	0.48
1:D:39:SER:O	1:D:43:THR:HG23	2.12	0.48
1:C:146:VAL:HG13	1:C:147:MET:HE2	1.95	0.48
1:D:30:ARG:HG2	1:D:64:GLU:HG2	1.95	0.48
1:D:43:THR:HB	1:D:49:ILE:HG12	1.95	0.48
1:A:248:THR:HG21	6:A:438:HOH:O	2.13	0.47
1:B:254:LYS:HG2	1:B:280:GLU:HG2	1.96	0.47
1:A:336:LEU:HD13	6:A:440:HOH:O	2.13	0.47
1:B:340:LYS:HG3	1:B:344:LEU:HD23	1.95	0.47
1:C:9:ILE:HG13	1:C:51:GLU:OE1	2.14	0.47
1:C:88:PRO:HD2	1:C:132:ASN:OD1	2.15	0.47
1:C:339:ASP:HB3	6:C:732:HOH:O	2.14	0.47
1:B:131:MET:HE3	1:C:91:ARG:HB3	1.97	0.47
1:A:257:LYS:NZ	6:A:611:HOH:O	2.49	0.46
1:A:17:LYS:NZ	1:A:54:ASN:O	2.39	0.46
1:C:223:ILE:HD11	6:C:547:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:N	1:B:275:LEU:HD12	2.31	0.46
1:C:51:GLU:HG3	1:C:52:ARG:N	2.31	0.46
1:A:239:VAL:CG2	1:A:256:VAL:CG1	2.92	0.45
1:A:281:TRP:CE3	1:A:284:GLY:HA2	2.51	0.45
1:C:219:LYS:HG2	6:C:506:HOH:O	2.15	0.45
1:C:17:LYS:NZ	1:C:54:ASN:O	2.48	0.45
1:D:33:ALA:HB3	1:D:62:VAL:CG2	2.46	0.45
1:C:137:PRO:HD2	1:C:140:ILE:HD12	1.98	0.45
1:D:346:LYS:HA	1:D:347:PRO:HD3	1.77	0.45
1:A:327:PHE:HA	1:A:351:LEU:CD2	2.47	0.45
1:D:80:ARG:HD3	6:D:666:HOH:O	2.15	0.45
1:B:148:ILE:N	1:B:149:PRO:CD	2.80	0.44
1:A:28:ILE:HB	1:A:67:GLU:HG3	1.99	0.44
1:B:148:ILE:HB	1:B:149:PRO:HD3	1.99	0.44
1:C:22:PRO:HG3	1:C:67:GLU:HG3	2.00	0.44
1:A:241:MET:HB3	6:A:438:HOH:O	2.18	0.44
1:D:83:VAL:O	1:D:149:PRO:HB3	2.18	0.44
1:D:228:MET:HE3	1:D:233:GLY:HA2	1.98	0.44
1:C:197:VAL:HG11	1:C:223:ILE:CD1	2.47	0.44
1:A:157:HIS:CG	1:A:296:PRO:HD3	2.53	0.44
1:D:26:ASP:OD1	1:D:127:ASN:HA	2.18	0.44
1:B:312:LYS:NZ	4:B:354:EDO:H21	2.33	0.43
1:D:171:VAL:HG23	1:D:236:VAL:HG11	1.98	0.43
1:D:30:ARG:HG2	1:D:64:GLU:CG	2.49	0.43
1:D:152:MET:CE	1:D:316:PRO:HG3	2.47	0.43
1:B:19:LYS:HE2	6:B:484:HOH:O	2.18	0.43
1:C:239:VAL:CG2	1:C:256:VAL:HG13	2.38	0.43
1:D:224:VAL:O	1:D:228:MET:HG2	2.19	0.43
1:D:200:ARG:NH2	1:D:341:PRO:O	2.52	0.43
1:C:148:ILE:N	1:C:149:PRO:CD	2.82	0.43
1:D:76:LYS:HB2	1:D:77:PRO:CD	2.49	0.43
1:D:267:TYR:CD1	1:D:267:TYR:C	2.92	0.42
1:B:264:ASN:O	1:B:292:GLY:HA2	2.19	0.42
1:D:17:LYS:NZ	1:D:54:ASN:O	2.52	0.42
1:C:346:LYS:HA	1:C:347:PRO:HD3	1.84	0.42
1:A:5:ALA:HB2	1:A:56:ILE:HA	2.01	0.42
1:B:110:TRP:CE2	1:B:114:ASN:HB2	2.54	0.42
1:C:219:LYS:C	1:C:221:GLY:N	2.72	0.42
1:D:136:LEU:HD12	1:D:137:PRO:HD2	2.01	0.42
1:D:148:ILE:N	1:D:149:PRO:CD	2.83	0.42
1:D:131:MET:HA	1:D:131:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:N	1:A:149:PRO:CD	2.83	0.41
1:C:254:LYS:HG2	1:C:280:GLU:HG2	2.02	0.41
1:D:267:TYR:C	1:D:267:TYR:HD1	2.24	0.41
1:A:200:ARG:HA	1:A:201:PRO:HD3	1.98	0.41
1:B:283:CYS:HB3	1:D:268:HIS:O	2.20	0.41
1:B:299:ARG:NE	4:B:358[B]:EDO:H11	2.35	0.41
1:B:340:LYS:HA	1:B:341:PRO:HD2	1.87	0.41
1:A:264:ASN:O	1:A:292:GLY:HA2	2.21	0.41
1:A:222:HIS:HE1	1:A:251:GLN:HG2	1.86	0.41
1:B:339:ASP:O	1:B:341:PRO:HD3	2.21	0.41
1:D:157:HIS:CG	1:D:296:PRO:HD3	2.56	0.41
1:D:223:ILE:HA	1:D:223:ILE:HD12	1.79	0.41
1:D:146:VAL:HG13	1:D:147:MET:HE2	2.03	0.41
1:A:7:LEU:O	1:A:53:HIS:HA	2.21	0.41
1:B:35:ALA:HA	1:B:36:PRO:HD3	1.84	0.41
1:D:228:MET:HE1	1:D:233:GLY:O	2.21	0.41
1:C:91:ARG:NH2	6:C:468:HOH:O	2.52	0.40
1:C:189:ARG:HA	1:C:189:ARG:HD2	1.92	0.40
1:D:189:ARG:HA	1:D:189:ARG:HD2	1.84	0.40
1:D:28:ILE:HB	1:D:67:GLU:HG2	2.02	0.40
1:B:200:ARG:HA	1:B:201:PRO:HD3	1.94	0.40
1:C:168:SER:HB2	1:C:237:ASP:OD2	2.20	0.40
1:A:135:HIS:O	1:A:137:PRO:HD3	2.22	0.40
1:C:241:MET:HG2	1:C:248:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	350/352 (99%)	335 (96%)	15 (4%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	350/352 (99%)	330 (94%)	20 (6%)	0	100	100
1	C	350/352 (99%)	331 (95%)	18 (5%)	1 (0%)	44	49
1	D	350/352 (99%)	332 (95%)	17 (5%)	1 (0%)	44	49
All	All	1400/1408 (99%)	1328 (95%)	70 (5%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	219	LYS
1	C	219	LYS

### 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	278/278 (100%)	277 (100%)	1 (0%)	93	97
1	B	278/278 (100%)	275 (99%)	3 (1%)	78	88
1	C	278/278 (100%)	272 (98%)	6 (2%)	57	70
1	D	278/278 (100%)	271 (98%)	7 (2%)	53	65
All	All	1112/1112 (100%)	1095 (98%)	17 (2%)	70	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	LEU
1	B	36	PRO
1	B	256	VAL
1	B	339	ASP
1	C	43	THR
1	C	146	VAL
1	C	218	TYR
1	C	232	ASN
1	C	256	VAL

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Mol	Chain	Res	Type
1	C	339	ASP
1	D	30	ARG
1	D	43	THR
1	D	76	LYS
1	D	256	VAL
1	D	267	TYR
1	D	338	LYS
1	D	339	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	B	135	HIS
1	C	42	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](#)

Of 27 ligands modelled in this entry, 10 are monoatomic - leaving 17 for Mogul analysis.

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	ACT	A	353	2	1,3,3	0.24	0	0,3,3	0.00	-
4	EDO	A	355	-	3,3,3	0.56	0	2,2,2	0.34	0
4	EDO	A	356	-	3,3,3	0.56	0	2,2,2	0.17	0
4	EDO	A	358	-	3,3,3	0.50	0	2,2,2	0.38	0
4	EDO	A	359	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	A	360	-	3,3,3	0.49	0	2,2,2	0.29	0
3	ACT	B	353	2	1,3,3	0.77	0	0,3,3	0.00	-
4	EDO	B	354	-	3,3,3	0.37	0	2,2,2	0.54	0
4	EDO	B	358[A]	-	3,3,3	0.48	0	2,2,2	0.47	0
4	EDO	B	358[B]	-	3,3,3	0.43	0	2,2,2	0.46	0
3	ACT	C	354	-	1,3,3	1.36	0	0,3,3	0.00	-
3	ACT	C	355	2	1,3,3	0.38	0	0,3,3	0.00	-
4	EDO	C	356	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	C	358[A]	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	C	358[B]	-	3,3,3	0.41	0	2,2,2	0.50	0
4	EDO	C	359	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	C	360	-	3,3,3	0.35	0	2,2,2	0.74	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	ACT	A	353	2	-	0/0/0/0	0/0/0/0
4	EDO	A	355	-	-	0/1/1/1	0/0/0/0
4	EDO	A	356	-	-	0/1/1/1	0/0/0/0
4	EDO	A	358	-	-	0/1/1/1	0/0/0/0
4	EDO	A	359	-	-	0/1/1/1	0/0/0/0
4	EDO	A	360	-	-	0/1/1/1	0/0/0/0
3	ACT	B	353	2	-	0/0/0/0	0/0/0/0
4	EDO	B	354	-	-	0/1/1/1	0/0/0/0
4	EDO	B	358[A]	-	-	0/1/1/1	0/0/0/0
4	EDO	B	358[B]	-	-	0/1/1/1	0/0/0/0
3	ACT	C	354	-	-	0/0/0/0	0/0/0/0
3	ACT	C	355	2	-	0/0/0/0	0/0/0/0
4	EDO	C	356	-	-	0/1/1/1	0/0/0/0
4	EDO	C	358[A]	-	-	0/1/1/1	0/0/0/0
4	EDO	C	358[B]	-	-	0/1/1/1	0/0/0/0
4	EDO	C	359	-	-	0/1/1/1	0/0/0/0
4	EDO	C	360	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
4	A	355	EDO	1	0
4	A	356	EDO	1	0
4	B	354	EDO	1	0
4	B	358[B]	EDO	2	0
4	C	356	EDO	1	0
4	C	360	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	352/352 (100%)	0.06	9 (2%) 56 54	24, 36, 59, 79	0
1	B	352/352 (100%)	0.08	8 (2%) 61 58	24, 37, 72, 104	0
1	C	352/352 (100%)	0.04	6 (1%) 70 68	27, 37, 61, 91	0
1	D	352/352 (100%)	0.35	30 (8%) 11 10	29, 45, 80, 116	0
All	All	1408/1408 (100%)	0.13	53 (3%) 41 39	24, 38, 69, 116	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	TYR	7.5
1	D	269	GLY	6.7
1	D	352	ALA	4.9
1	D	7	LEU	4.4
1	B	271	GLY	4.4
1	D	271	GLY	4.3
1	D	53	HIS	3.4
1	D	275	LEU	3.4
1	B	352	ALA	3.3
1	A	11	LYS	3.1
1	B	45	PHE	3.1
1	A	7	LEU	3.0
1	D	232	ASN	3.0
1	A	53	HIS	3.0
1	D	246	SER	3.0
1	D	221	GLY	3.0
1	D	47	GLY	3.0
1	D	339	ASP	3.0
1	B	273	ALA	2.9
1	D	51	GLU	2.9
1	A	12	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	2.8
1	D	229	LYS	2.8
1	D	270	SER	2.8
1	A	220	ASN	2.7
1	A	218	TYR	2.7
1	D	219	LYS	2.7
1	A	352	ALA	2.7
1	A	9	ILE	2.6
1	C	246	SER	2.6
1	B	272	ASP	2.6
1	D	273	ALA	2.6
1	D	199	SER	2.6
1	D	341	PRO	2.6
1	B	270	SER	2.5
1	D	220	ASN	2.5
1	B	275	LEU	2.4
1	A	246	SER	2.4
1	D	272	ASP	2.4
1	B	53	HIS	2.4
1	D	222	HIS	2.4
1	D	248	THR	2.3
1	C	223	ILE	2.3
1	D	223	ILE	2.2
1	D	9	ILE	2.2
1	D	50	GLY	2.2
1	D	224	VAL	2.2
1	C	271	GLY	2.2
1	C	222	HIS	2.1
1	D	54	ASN	2.1
1	D	342	LYS	2.1
1	C	218	TYR	2.1
1	D	201	PRO	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 ⓘ

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
4	EDO	A	358	4/4	0.95	0.34	18.35	48,53,58,62	0
4	EDO	B	358[A]	4/4	0.85	0.46	16.65	34,34,35,35	4
3	ACT	C	355	4/4	0.96	0.28	10.52	40,42,46,47	0
4	EDO	B	358[B]	4/4	0.85	0.46	10.47	22,30,31,31	4
4	EDO	A	360	4/4	0.92	0.23	7.32	60,62,64,68	0
4	EDO	A	356	4/4	0.86	0.27	6.91	42,57,57,62	0
4	EDO	C	356	4/4	0.89	0.18	6.79	60,64,66,66	0
4	EDO	C	360	4/4	0.91	0.30	5.72	41,54,58,67	0
4	EDO	C	359	4/4	0.88	0.20	3.11	71,71,76,79	0
4	EDO	A	355	4/4	0.91	0.15	2.50	37,45,47,51	0
3	ACT	A	353	4/4	0.95	0.17	2.11	27,33,35,39	0
3	ACT	B	353	4/4	0.95	0.20	1.56	37,39,40,41	0
4	EDO	B	354	4/4	0.96	0.14	1.05	52,52,55,56	0
2	ZN	B	355	1/1	1.00	0.10	-0.95	36,36,36,36	0
2	ZN	C	353	1/1	1.00	0.09	-1.56	38,38,38,38	0
2	ZN	A	354	1/1	0.99	0.09	-1.75	36,36,36,36	0
2	ZN	D	357	1/1	1.00	0.07	-2.39	44,44,44,44	0
5	CL	B	359	1/1	0.85	0.25	-	79,79,79,79	0
3	ACT	C	354	4/4	0.60	0.70	-	123,124,124,125	0
4	EDO	C	358[B]	4/4	0.88	0.77	-	37,40,44,47	4
4	EDO	C	358[A]	4/4	0.88	0.77	-	35,37,38,46	4
5	CL	C	357	1/1	0.90	0.34	-	77,77,77,77	0
4	EDO	A	359	4/4	0.54	0.19	-	86,90,92,93	0
5	CL	A	357	1/1	0.88	0.22	-	87,87,87,87	0
5	CL	B	360	1/1	0.93	0.07	-	70,70,70,70	0
5	CL	B	356	1/1	0.93	0.10	-	80,80,80,80	0
5	CL	D	353	1/1	0.97	0.24	-	82,82,82,82	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.