Full wwPDB X-ray Structure Validation Report (i)

Mar 19, 2025 – 11:35 AM EDT

PDB ID	:	3OKS
Title	:	Crystal structure of 4-aminobutyrate transaminase from mycobacterium smegmatis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2010-08-25
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

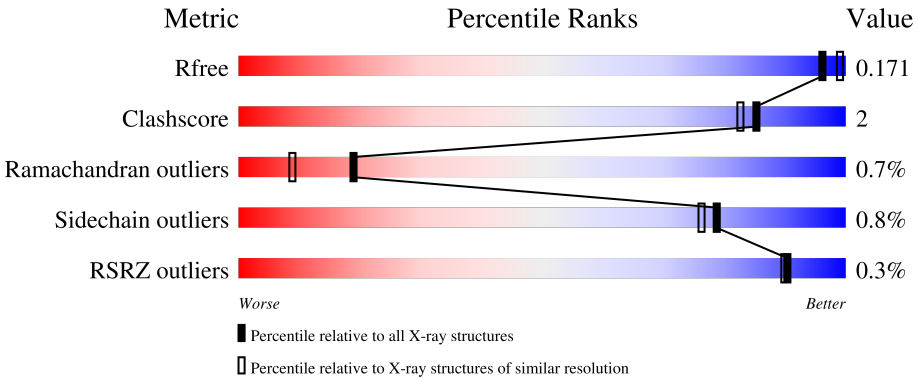
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	451	93% 5% •
1	B	451	94% • •
1	C	451	94% • •
1	D	451	93% 6% •

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
1	LLP	A	292[B]	-	X	-	-
1	LLP	B	292[B]	-	X	-	-
1	LLP	C	292[B]	-	X	-	-
1	LLP	D	292[B]	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14977 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.

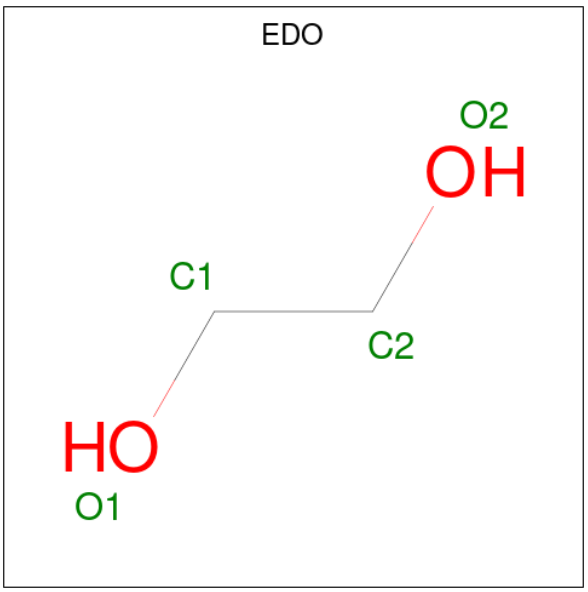
- Molecule 1 is a protein called 4-aminobutyrate transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	P	S	0	13	0
			3351	2104	594	635	1	17			
1	B	445	Total	C	N	O	P	S	0	14	0
			3348	2106	581	645	1	15			
1	C	447	Total	C	N	O	P	S	0	8	0
			3321	2085	582	635	1	18			
1	D	447	Total	C	N	O	P	S	0	9	0
			3339	2093	589	640	1	16			

There are 20 discrepancies between the modelled and reference sequences:

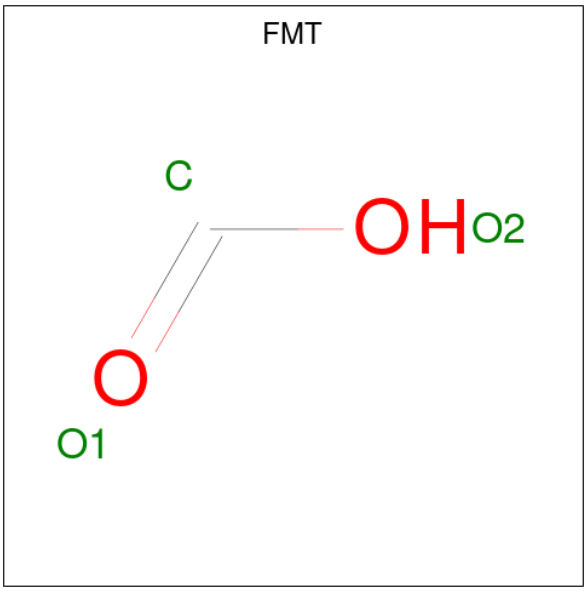
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0QWJ0
A	-2	PRO	-	expression tag	UNP A0QWJ0
A	-1	GLY	-	expression tag	UNP A0QWJ0
A	0	SER	-	expression tag	UNP A0QWJ0
A	2	VAL	-	expression tag	UNP A0QWJ0
B	-3	GLY	-	expression tag	UNP A0QWJ0
B	-2	PRO	-	expression tag	UNP A0QWJ0
B	-1	GLY	-	expression tag	UNP A0QWJ0
B	0	SER	-	expression tag	UNP A0QWJ0
B	2	VAL	-	expression tag	UNP A0QWJ0
C	-3	GLY	-	expression tag	UNP A0QWJ0
C	-2	PRO	-	expression tag	UNP A0QWJ0
C	-1	GLY	-	expression tag	UNP A0QWJ0
C	0	SER	-	expression tag	UNP A0QWJ0
C	2	VAL	-	expression tag	UNP A0QWJ0
D	-3	GLY	-	expression tag	UNP A0QWJ0
D	-2	PRO	-	expression tag	UNP A0QWJ0
D	-1	GLY	-	expression tag	UNP A0QWJ0
D	0	SER	-	expression tag	UNP A0QWJ0
D	2	VAL	-	expression tag	UNP A0QWJ0

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



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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

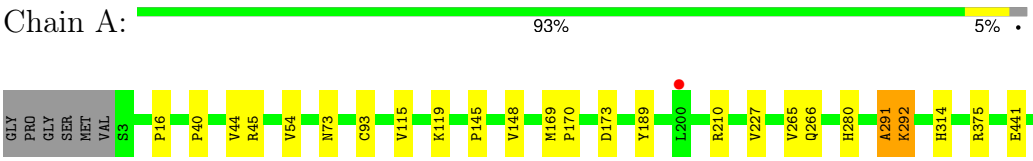
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	374	Total O 375 375	0	3
5	B	399	Total O 399 399	0	2
5	C	366	Total O 368 368	0	3
5	D	402	Total O 403 403	0	5

3 Residue-property plots (i)

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

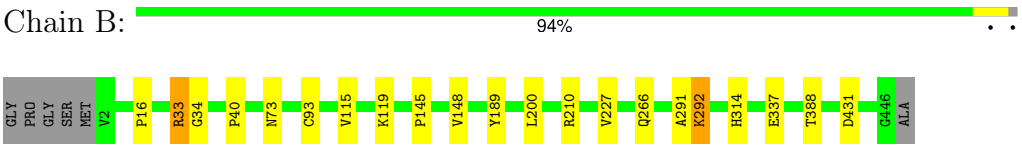
• Molecule 1: 4-aminobutyrate transaminase

Chain A:



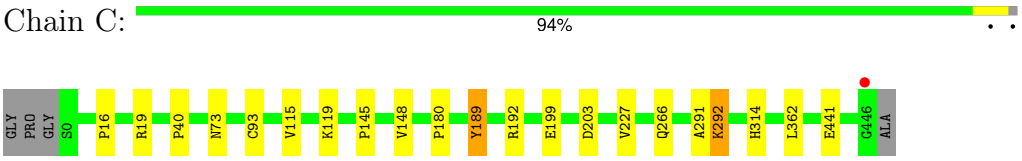
• Molecule 1: 4-aminobutyrate transaminase

Chain B:



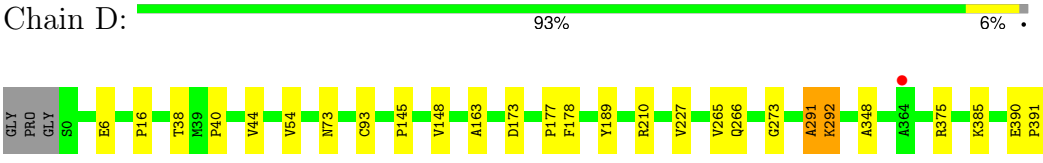
• Molecule 1: 4-aminobutyrate transaminase

Chain C:



• Molecule 1: 4-aminobutyrate transaminase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	128.01Å 128.01Å 104.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 1.80 48.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.20-1.80) 99.9 (48.20-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.126 , 0.159 0.138 , 0.171	Depositor DCC
R_{free} test set	7782 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, LLP, FMT, MG

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	0.64	0/3416	0.70	0/4638
1	B	0.67	0/3415	0.71	1/4642 (0.0%)
1	C	0.69	0/3370	0.70	1/4581 (0.0%)
1	D	0.72	0/3390	0.76	2/4605 (0.0%)
All	All	0.68	0/13591	0.72	4/18466 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	375[A]	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	D	375[B]	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	431	ASP	CB-CG-OD1	6.01	123.70	118.30
1	C	19	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3351	0	3352	21	0
1	B	3348	0	3340	12	0
1	C	3321	0	3300	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3339	0	3327	16	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	12	0	18	2	0
3	A	9	0	3	0	0
3	B	12	0	4	0	0
3	C	6	0	2	0	0
3	D	9	0	3	0	0
4	C	1	0	0	0	0
5	A	375	0	0	3	1
5	B	399	0	0	2	0
5	C	368	0	0	0	1
5	D	403	0	0	3	0
All	All	14977	0	13385	57	1

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 2.

All (57) 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:A:280[B]:HIS:NE2	1:A:375[B]:ARG:NH1	1.82	1.27
1:A:280[B]:HIS:CE1	1:A:375[B]:ARG:NH1	2.28	1.01
1:A:280[B]:HIS:CD2	1:A:375[B]:ARG:NH1	2.37	0.92
1:A:280[B]:HIS:CD2	1:A:375[B]:ARG:CZ	2.53	0.91
1:C:362:LEU:HD11	1:C:441:GLU:HG2	1.61	0.81
1:B:337[B]:GLU:OE1	5:B:1534:HOH:O	2.01	0.78
1:A:280[B]:HIS:CE1	1:A:375[B]:ARG:HH12	1.95	0.76
1:D:210:ARG:NH1	5:D:529:HOH:O	2.21	0.73
1:B:148:VAL:CG1	1:B:227:VAL:HG22	2.23	0.68
1:A:280[B]:HIS:NE2	1:A:375[B]:ARG:CZ	2.57	0.66
1:A:45[A]:ARG:NH1	5:A:1046:HOH:O	2.30	0.65
1:D:441:GLU:OE2	5:D:1373:HOH:O	2.16	0.61
1:A:441:GLU:OE2	5:A:615:HOH:O	2.17	0.57
1:C:362:LEU:CD1	1:C:441:GLU:HG2	2.31	0.56
1:A:115:VAL:HB	1:A:119:LYS:HD3	1.89	0.54
1:A:280[B]:HIS:CD2	1:A:375[B]:ARG:NH2	2.75	0.54
1:B:115:VAL:HB	1:B:119:LYS:HD3	1.89	0.54
1:D:38:THR:HG23	2:D:485:EDO:H11	1.90	0.53
1:B:200:LEU:HD11	1:B:210:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:HB3	1:B:314[B]:HIS:CE1	2.45	0.51
1:B:16:PRO:HB3	1:B:40:PRO:O	2.10	0.51
1:A:169[A]:MET:HE3	1:A:170:PRO:HA	1.92	0.51
1:C:16:PRO:HB3	1:C:40:PRO:O	2.11	0.50
1:C:266:GLN:HA	1:C:292[B]:LLP:HD3	1.94	0.50
1:C:314[B]:HIS:CE1	1:D:173:ASP:HB3	2.47	0.49
1:B:200:LEU:HD11	1:B:210:ARG:HH12	1.78	0.48
1:D:44:VAL:CG1	1:D:54:VAL:HG12	2.44	0.48
1:D:266:GLN:HA	1:D:292[B]:LLP:HD3	1.95	0.48
1:A:314[B]:HIS:CD2	5:A:1508:HOH:O	2.67	0.48
1:C:148:VAL:CG1	1:C:227:VAL:HG22	2.45	0.47
1:D:292[A]:LLP:NZ	1:D:292[A]:LLP:O3	2.47	0.47
1:A:16:PRO:HB3	1:A:40:PRO:O	2.15	0.47
1:C:292[A]:LLP:O3	1:C:292[A]:LLP:NZ	2.47	0.47
1:B:266:GLN:HA	1:B:292[B]:LLP:HD3	1.95	0.47
1:D:265:VAL:HG13	1:D:291:ALA:HB3	1.98	0.46
1:B:292[A]:LLP:O3	1:B:292[A]:LLP:NZ	2.46	0.46
1:C:199:GLU:O	1:C:203:ASP:HB3	2.16	0.46
1:B:148:VAL:HG11	1:B:227:VAL:HG22	1.97	0.45
1:C:115:VAL:HB	1:C:119:LYS:HD3	2.00	0.44
1:C:180:PRO:HG2	1:D:177:PRO:HB2	1.99	0.43
1:C:189:TYR:CE2	1:C:192:ARG:HD2	2.53	0.43
1:D:16:PRO:HB3	1:D:40:PRO:O	2.18	0.43
1:A:292[A]:LLP:O3	1:A:292[A]:LLP:NZ	2.46	0.43
1:D:6:GLU:HG2	5:D:1376:HOH:O	2.19	0.42
1:A:265:VAL:HG13	1:A:291:ALA:HB3	2.02	0.42
1:D:163:ALA:HB2	1:D:178:PHE:HB3	2.02	0.42
1:D:273:GLY:HA2	1:D:348:ALA:HB3	2.02	0.42
1:A:44:VAL:CG1	1:A:54:VAL:HG12	2.50	0.41
1:A:148:VAL:CG1	1:A:227:VAL:HG22	2.50	0.41
1:B:388:THR:HB	5:B:473:HOH:O	2.19	0.41
1:A:280[B]:HIS:CE1	1:A:375[B]:ARG:HH11	2.27	0.41
1:B:33:ARG:HG3	1:B:34:GLY:N	2.36	0.41
1:A:210[A]:ARG:HB3	1:A:210[A]:ARG:CZ	2.51	0.40
1:D:148:VAL:CG1	1:D:227:VAL:HG22	2.51	0.40
1:A:266:GLN:HA	1:A:292[B]:LLP:HD3	2.04	0.40
1:D:412:SER:OG	2:D:485:EDO:H22	2.21	0.40
1:D:385:LYS:HD2	1:D:390:GLU:CD	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1479:HOH:O	5:C:1478:HOH:O[4_565]	2.02	0.18

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	453/451 (100%)	433 (96%)	17 (4%)	3 (1%)	19	9
1	B	455/451 (101%)	437 (96%)	15 (3%)	3 (1%)	19	9
1	C	451/451 (100%)	434 (96%)	14 (3%)	3 (1%)	19	9
1	D	452/451 (100%)	433 (96%)	16 (4%)	3 (1%)	19	9
All	All	1811/1804 (100%)	1737 (96%)	62 (3%)	12 (1%)	19	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	291	ALA
1	D	93	CYS
1	D	291	ALA
1	A	93	CYS
1	A	291	ALA
1	B	291	ALA
1	C	93	CYS
1	B	145	PRO
1	B	93	CYS
1	C	145	PRO
1	D	145	PRO
1	A	145	PRO

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	343/341 (101%)	341 (99%)	2 (1%)	84	82
1	B	345/341 (101%)	342 (99%)	3 (1%)	75	72
1	C	338/341 (99%)	336 (99%)	2 (1%)	84	82
1	D	341/341 (100%)	338 (99%)	3 (1%)	75	72
All	All	1367/1364 (100%)	1357 (99%)	10 (1%)	79	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	189	TYR
1	B	33	ARG
1	B	73	ASN
1	B	189	TYR
1	C	73	ASN
1	C	189	TYR
1	D	73	ASN
1	D	189	TYR
1	D	391	PRO

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

Mol	Chain	Res	Type
1	A	233	GLN
1	A	266	GLN
1	B	233	GLN
1	B	266	GLN
1	C	233	GLN
1	C	266	GLN
1	D	233	GLN
1	D	266	GLN
1	D	349	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	C	292[B]	-	23,8,25	12.29	5 (21%)	25,8,34	3.68	5 (20%)
1	LLP	C	292[A]	-	23,24,25	2.10	7 (30%)	25,32,34	1.76	4 (16%)
1	LLP	B	292[B]	-	23,8,25	12.62	5 (21%)	25,8,34	3.75	8 (32%)
1	LLP	A	292[A]	-	23,24,25	1.94	7 (30%)	25,32,34	1.90	5 (20%)
1	LLP	A	292[B]	-	23,8,25	12.90	5 (21%)	25,8,34	4.14	6 (24%)
1	LLP	B	292[A]	-	23,24,25	2.11	7 (30%)	25,32,34	1.93	7 (28%)
1	LLP	D	292[A]	-	23,24,25	2.01	7 (30%)	25,32,34	1.82	4 (16%)
1	LLP	D	292[B]	-	23,8,25	13.00	5 (21%)	25,8,34	3.68	5 (20%)

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
1	LLP	C	292[B]	-	-	3/16/7/19	0/1/0/1
1	LLP	C	292[A]	-	-	3/16/17/19	0/1/1/1
1	LLP	B	292[B]	-	-	4/16/7/19	0/1/0/1
1	LLP	A	292[A]	-	-	3/16/17/19	0/1/1/1
1	LLP	A	292[B]	-	-	5/16/7/19	0/1/0/1
1	LLP	B	292[A]	-	-	3/16/17/19	0/1/1/1
1	LLP	D	292[A]	-	-	3/16/17/19	0/1/1/1
1	LLP	D	292[B]	-	-	4/16/7/19	0/1/0/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	292[B]	LLP	C4'-NZ	61.88	3.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292[B]	LLP	C4'-NZ	61.39	3.32	1.27
1	B	292[B]	LLP	C4'-NZ	59.98	3.28	1.27
1	C	292[B]	LLP	C4'-NZ	58.43	3.22	1.27
1	D	292[A]	LLP	O3-C3	-5.66	1.24	1.36
1	D	292[B]	LLP	O3-C3	-5.66	1.24	1.36
1	B	292[A]	LLP	O3-C3	-5.23	1.24	1.36
1	B	292[B]	LLP	O3-C3	-5.23	1.24	1.36
1	A	292[A]	LLP	O3-C3	-4.89	1.25	1.36
1	A	292[B]	LLP	O3-C3	-4.89	1.25	1.36
1	C	292[A]	LLP	O3-C3	-4.88	1.25	1.36
1	C	292[B]	LLP	O3-C3	-4.88	1.25	1.36
1	B	292[A]	LLP	CE-NZ	4.32	1.56	1.46
1	C	292[A]	LLP	CE-NZ	4.23	1.56	1.46
1	D	292[A]	LLP	CE-NZ	3.66	1.55	1.46
1	A	292[A]	LLP	CE-NZ	3.66	1.55	1.46
1	C	292[A]	LLP	C4'-NZ	3.59	1.39	1.27
1	C	292[A]	LLP	C6-N1	3.59	1.41	1.34
1	C	292[B]	LLP	C6-N1	3.59	1.41	1.34
1	A	292[A]	LLP	C6-N1	3.49	1.41	1.34
1	A	292[B]	LLP	C6-N1	3.49	1.41	1.34
1	B	292[A]	LLP	C4'-NZ	3.42	1.38	1.27
1	B	292[A]	LLP	C6-N1	3.35	1.41	1.34
1	B	292[B]	LLP	C6-N1	3.35	1.41	1.34
1	D	292[A]	LLP	C4'-NZ	3.30	1.38	1.27
1	B	292[A]	LLP	C2-N1	3.02	1.39	1.33
1	B	292[B]	LLP	C2-N1	3.02	1.39	1.33
1	C	292[A]	LLP	C2-N1	2.92	1.39	1.33
1	C	292[B]	LLP	C2-N1	2.92	1.39	1.33
1	D	292[A]	LLP	C6-N1	2.90	1.40	1.34
1	D	292[B]	LLP	C6-N1	2.90	1.40	1.34
1	A	292[A]	LLP	C4'-NZ	2.84	1.36	1.27
1	A	292[A]	LLP	C2-N1	2.82	1.38	1.33
1	A	292[B]	LLP	C2-N1	2.82	1.38	1.33
1	B	292[A]	LLP	C4-C4'	2.70	1.52	1.46
1	B	292[B]	LLP	C4-C4'	2.70	1.52	1.46
1	C	292[A]	LLP	CD-CE	2.68	1.60	1.51
1	D	292[A]	LLP	C4-C4'	2.66	1.52	1.46
1	D	292[B]	LLP	C4-C4'	2.66	1.52	1.46
1	D	292[A]	LLP	C2-N1	2.58	1.38	1.33
1	D	292[B]	LLP	C2-N1	2.58	1.38	1.33
1	A	292[A]	LLP	C4-C4'	2.53	1.52	1.46
1	A	292[B]	LLP	C4-C4'	2.53	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292[A]	LLP	C4-C4'	2.48	1.51	1.46
1	C	292[B]	LLP	C4-C4'	2.48	1.51	1.46
1	A	292[A]	LLP	CD-CE	2.48	1.60	1.51
1	D	292[A]	LLP	CD-CE	2.21	1.59	1.51
1	B	292[A]	LLP	CD-CE	2.12	1.58	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292[B]	LLP	CE-NZ-C4'	-18.28	60.16	118.72
1	C	292[B]	LLP	CE-NZ-C4'	-16.18	66.89	118.72
1	B	292[B]	LLP	CE-NZ-C4'	-16.13	67.06	118.72
1	D	292[B]	LLP	CE-NZ-C4'	-15.94	67.68	118.72
1	A	292[A]	LLP	OP4-C5'-C5	6.48	121.50	109.36
1	A	292[B]	LLP	OP4-C5'-C5	6.48	121.50	109.36
1	D	292[A]	LLP	OP4-C5'-C5	5.89	120.40	109.36
1	D	292[B]	LLP	OP4-C5'-C5	5.89	120.40	109.36
1	C	292[A]	LLP	OP4-C5'-C5	5.72	120.08	109.36
1	C	292[B]	LLP	OP4-C5'-C5	5.72	120.08	109.36
1	B	292[A]	LLP	OP4-C5'-C5	5.29	119.27	109.36
1	B	292[B]	LLP	OP4-C5'-C5	5.29	119.27	109.36
1	A	292[B]	LLP	C4-C4'-NZ	4.28	143.77	124.04
1	D	292[B]	LLP	C4-C4'-NZ	4.14	143.15	124.04
1	B	292[B]	LLP	C4-C4'-NZ	3.96	142.32	124.04
1	D	292[A]	LLP	C4-C4'-NZ	-3.91	106.00	124.04
1	C	292[B]	LLP	C4-C4'-NZ	3.90	142.02	124.04
1	A	292[A]	LLP	C4-C4'-NZ	-3.79	106.56	124.04
1	B	292[A]	LLP	C4-C4'-NZ	-3.76	106.68	124.04
1	C	292[A]	LLP	C4-C4'-NZ	-3.70	106.95	124.04
1	B	292[A]	LLP	OP3-P-OP2	3.26	120.04	107.80
1	B	292[B]	LLP	OP3-P-OP2	3.26	120.04	107.80
1	B	292[A]	LLP	C5-C6-N1	-3.14	118.72	123.83
1	B	292[B]	LLP	C5-C6-N1	-3.14	118.72	123.83
1	C	292[A]	LLP	OP3-P-OP2	2.80	118.29	107.80
1	C	292[B]	LLP	OP3-P-OP2	2.80	118.29	107.80
1	D	292[A]	LLP	OP3-P-OP2	2.61	117.57	107.80
1	D	292[B]	LLP	OP3-P-OP2	2.61	117.57	107.80
1	D	292[A]	LLP	OP2-P-OP4	-2.46	100.27	106.67
1	D	292[B]	LLP	OP2-P-OP4	-2.46	100.27	106.67
1	A	292[A]	LLP	OP2-P-OP4	-2.37	100.48	106.67
1	A	292[B]	LLP	OP2-P-OP4	-2.37	100.48	106.67
1	A	292[A]	LLP	OP3-P-OP2	2.37	116.69	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	292[B]	LLP	OP3-P-OP2	2.37	116.69	107.80
1	B	292[A]	LLP	O3-C3-C2	2.35	122.45	117.58
1	B	292[B]	LLP	O3-C3-C2	2.35	122.45	117.58
1	B	292[A]	LLP	OP2-P-OP4	-2.34	100.56	106.67
1	B	292[B]	LLP	OP2-P-OP4	-2.34	100.56	106.67
1	A	292[A]	LLP	O3-C3-C2	2.27	122.29	117.58
1	A	292[B]	LLP	O3-C3-C2	2.27	122.29	117.58
1	C	292[A]	LLP	OP2-P-OP4	-2.15	101.07	106.67
1	C	292[B]	LLP	OP2-P-OP4	-2.15	101.07	106.67
1	B	292[A]	LLP	C6-C5-C4	2.01	121.67	118.21
1	B	292[B]	LLP	C6-C5-C4	2.01	121.67	118.21

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	292[A]	LLP	CG-CD-CE-NZ
1	A	292[B]	LLP	C4-C4'-NZ-CE
1	A	292[B]	LLP	O-C-CA-CB
1	B	292[A]	LLP	CG-CD-CE-NZ
1	B	292[B]	LLP	C4-C4'-NZ-CE
1	C	292[A]	LLP	CG-CD-CE-NZ
1	C	292[B]	LLP	C4-C4'-NZ-CE
1	D	292[A]	LLP	CG-CD-CE-NZ
1	D	292[B]	LLP	C4-C4'-NZ-CE
1	B	292[A]	LLP	C4-C4'-NZ-CE
1	C	292[A]	LLP	C4-C4'-NZ-CE
1	A	292[A]	LLP	C4-C4'-NZ-CE
1	D	292[A]	LLP	C4-C4'-NZ-CE
1	A	292[B]	LLP	C3-C4-C4'-NZ
1	D	292[B]	LLP	C3-C4-C4'-NZ
1	B	292[B]	LLP	C3-C4-C4'-NZ
1	D	292[B]	LLP	C5-C4-C4'-NZ
1	C	292[A]	LLP	C3-C4-C4'-NZ
1	B	292[B]	LLP	C5-C4-C4'-NZ
1	A	292[A]	LLP	C3-C4-C4'-NZ
1	B	292[A]	LLP	C3-C4-C4'-NZ
1	C	292[B]	LLP	C3-C4-C4'-NZ
1	D	292[A]	LLP	C3-C4-C4'-NZ
1	A	292[B]	LLP	C5-C4-C4'-NZ
1	C	292[B]	LLP	C5-C4-C4'-NZ
1	A	292[B]	LLP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	292[B]	LLP	C-CA-CB-CG
1	D	292[B]	LLP	C-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	292[B]	LLP	1	0
1	C	292[A]	LLP	1	0
1	B	292[B]	LLP	1	0
1	A	292[A]	LLP	1	0
1	A	292[B]	LLP	1	0
1	B	292[A]	LLP	1	0
1	D	292[A]	LLP	1	0
1	D	292[B]	LLP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	FMT	C	460	-	2,2,2	0.53	0	1,1,1	0.37	0
3	FMT	D	465	-	2,2,2	0.58	0	1,1,1	0.37	0
3	FMT	A	460	-	2,2,2	0.71	0	1,1,1	0.39	0
3	FMT	C	465	-	2,2,2	0.55	0	1,1,1	0.38	0
3	FMT	B	460	-	2,2,2	0.57	0	1,1,1	0.32	0
2	EDO	A	455	-	3,3,3	0.40	0	2,2,2	0.17	0
2	EDO	A	480	-	3,3,3	0.48	0	2,2,2	0.11	0
2	EDO	C	480	-	3,3,3	0.51	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FMT	B	470	-	2,2,2	0.94	0	1,1,1	0.01	0
2	EDO	B	480	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	D	455	-	3,3,3	0.50	0	2,2,2	0.33	0
2	EDO	D	485	-	3,3,3	0.68	0	2,2,2	1.08	0
3	FMT	D	470	-	2,2,2	0.74	0	1,1,1	0.06	0
2	EDO	D	480	-	3,3,3	0.43	0	2,2,2	0.28	0
2	EDO	C	455	-	3,3,3	0.50	0	2,2,2	0.15	0
3	FMT	B	475	-	2,2,2	0.74	0	1,1,1	0.53	0
3	FMT	A	470	-	2,2,2	0.73	0	1,1,1	0.16	0
2	EDO	B	455	-	3,3,3	0.35	0	2,2,2	0.44	0
3	FMT	A	465	-	2,2,2	0.73	0	1,1,1	0.45	0
3	FMT	B	465	-	2,2,2	0.71	0	1,1,1	0.35	0
3	FMT	D	460	-	2,2,2	0.84	0	1,1,1	0.43	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	EDO	B	455	-	-	1/1/1/1	-
2	EDO	D	485	-	-	1/1/1/1	-
2	EDO	A	455	-	-	0/1/1/1	-
2	EDO	A	480	-	-	0/1/1/1	-
2	EDO	D	480	-	-	1/1/1/1	-
2	EDO	C	455	-	-	1/1/1/1	-
2	EDO	C	480	-	-	0/1/1/1	-
2	EDO	B	480	-	-	0/1/1/1	-
2	EDO	D	455	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	455	EDO	O1-C1-C2-O2
2	D	485	EDO	O1-C1-C2-O2
2	D	480	EDO	O1-C1-C2-O2
2	B	455	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	485	EDO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	443/451 (98%)	-0.78	2 (0%) 87 87	5, 11, 25, 43	12 (2%)
1	B	444/451 (98%)	-0.83	0 100 100	4, 10, 23, 39	13 (2%)
1	C	446/451 (98%)	-0.81	1 (0%) 92 91	5, 10, 26, 40	7 (1%)
1	D	446/451 (98%)	-0.91	2 (0%) 89 88	4, 8, 19, 34	8 (1%)
All	All	1779/1804 (98%)	-0.83	5 (0%) 90 90	4, 10, 24, 43	40 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	446	GLY	3.0
1	A	200	LEU	2.9
1	D	364	ALA	2.2
1	C	446	GLY	2.2
1	A	446	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	C	292[A]	24/25	0.95	0.07	4,8,12,15	21
1	LLP	C	292[B]	9/25	0.95	0.07	3,7,8,9	6
1	LLP	D	292[A]	24/25	0.95	0.07	3,7,13,15	21
1	LLP	D	292[B]	9/25	0.95	0.07	3,5,6,7	6
1	LLP	A	292[A]	24/25	0.96	0.07	3,9,13,16	21
1	LLP	A	292[B]	9/25	0.96	0.07	4,7,9,9	6
1	LLP	B	292[A]	24/25	0.96	0.07	4,9,12,16	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	B	292[B]	9/25	0.96	0.07	7,8,9,9	6

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	A	470	3/3	0.73	0.17	32,32,34,34	0
3	FMT	B	470	3/3	0.81	0.14	25,25,27,27	0
3	FMT	D	470	3/3	0.82	0.14	29,29,30,31	0
3	FMT	D	465	3/3	0.85	0.14	36,36,37,38	0
3	FMT	C	465	3/3	0.85	0.12	32,32,33,33	0
3	FMT	A	465	3/3	0.88	0.13	39,39,39,39	0
2	EDO	D	485	4/4	0.88	0.12	18,24,25,29	0
3	FMT	C	460	3/3	0.89	0.08	24,24,24,25	0
3	FMT	B	475	3/3	0.89	0.10	32,32,32,34	0
2	EDO	C	480	4/4	0.90	0.12	30,32,33,34	0
2	EDO	B	480	4/4	0.90	0.11	34,36,37,37	0
3	FMT	B	460	3/3	0.92	0.09	26,26,26,27	0
3	FMT	A	460	3/3	0.93	0.08	22,22,24,24	0
2	EDO	A	480	4/4	0.93	0.08	26,26,27,27	0
2	EDO	D	480	4/4	0.94	0.08	25,27,28,29	0
3	FMT	B	465	3/3	0.94	0.07	34,34,35,35	0
3	FMT	D	460	3/3	0.95	0.07	20,20,20,20	0
2	EDO	A	455	4/4	0.97	0.06	14,14,15,15	0
2	EDO	D	455	4/4	0.97	0.06	12,15,15,15	0
2	EDO	B	455	4/4	0.98	0.03	11,13,13,13	0
2	EDO	C	455	4/4	0.98	0.06	13,15,15,15	0
4	MG	C	448	1/1	0.99	0.08	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.