



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:02 PM BST

PDB ID : 5Y0S
Title : Crystal structure of apo Thermotoga maritima TmcAL(Form II)
Authors : Yamashita, S.; Tomita, K.
Deposited on : 2017-07-18
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

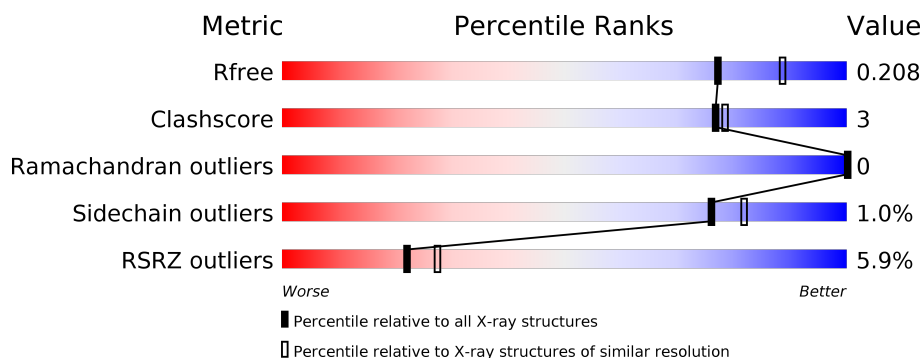
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 $\leq 5\%$. 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	425	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 94% 6% </div> </div>
1	B	425	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 5% 87% 12% </div> </div>
1	C	425	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 2% 92% 7% </div> </div>
1	D	425	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 15% 92% 7% </div> </div>

2 Entry composition [i](#)

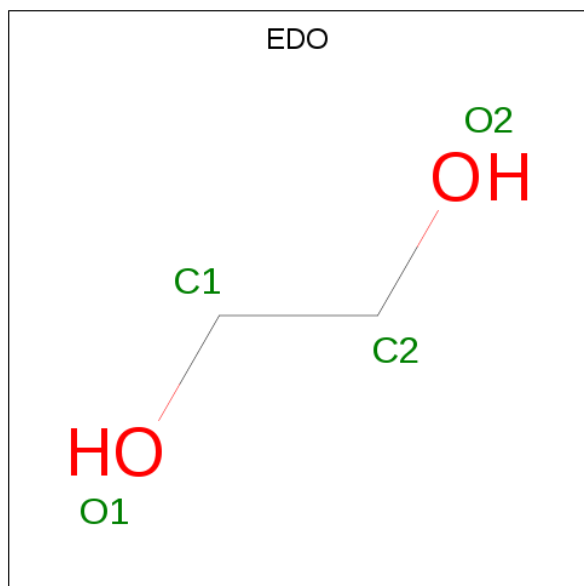
There are 3 unique types of molecules in this entry. The entry contains 14558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 *Thermotoga maritima* TmcAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3462	2222	598	624	18			
1	B	423	Total	C	N	O	S	0	0	0
			3462	2222	598	624	18			
1	C	423	Total	C	N	O	S	0	0	0
			3462	2222	598	624	18			
1	D	423	Total	C	N	O	S	0	0	0
			3462	2222	598	624	18			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total 186	O 186	0	0
3	B	121	Total 121	O 121	0	0
3	C	176	Total 176	O 176	0	0
3	D	139	Total 139	O 139	0	0

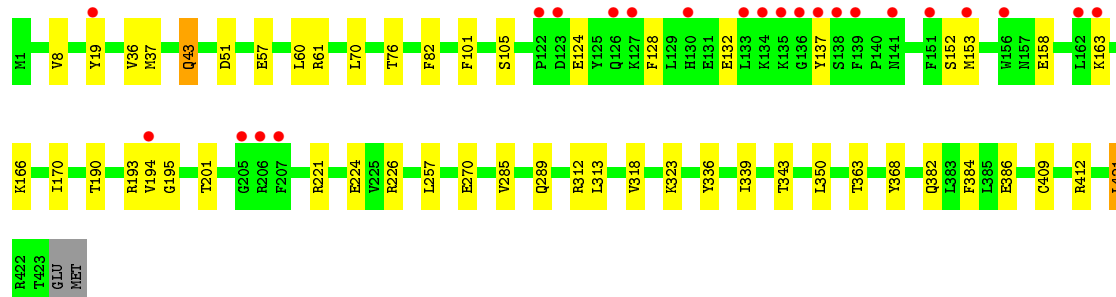
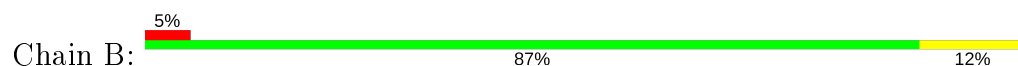
3 Residue-property plots [i](#)

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.

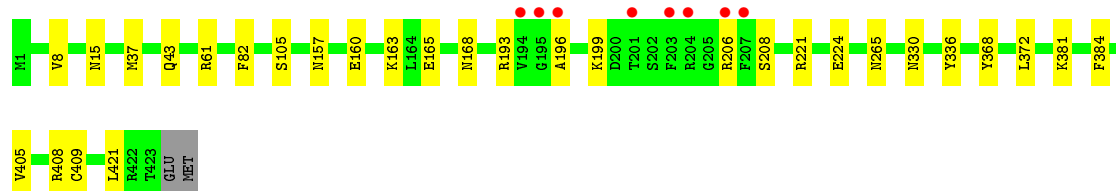
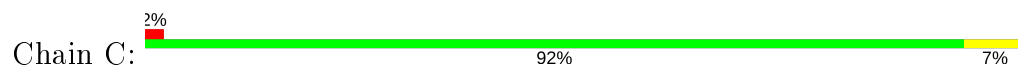
- Molecule 1: *Thermotoga maritima* TmcAL



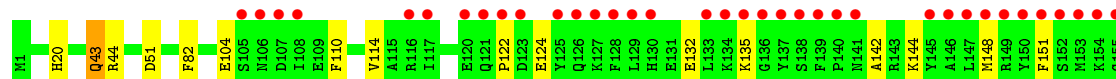
- Molecule 1: *Thermotoga maritima* TmcAL

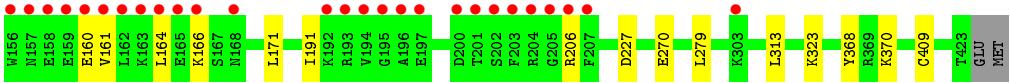


- Molecule 1: *Thermotoga maritima* TmcAL



- Molecule 1: *Thermotoga maritima* TmcAL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.99 Å 97.95 Å 144.28 Å 90.00° 99.18° 90.00°	Depositor
Resolution (Å)	49.89 – 2.10 49.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.89-2.10) 99.7 (49.89-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.10 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.169 , 0.207 0.171 , 0.208	Depositor DCC
R_{free} test set	6445 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14558	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CSD, CME, 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	0.43	0/3517	0.53	0/4723
1	B	0.37	0/3517	0.50	0/4723
1	C	0.42	0/3517	0.53	0/4723
1	D	0.38	0/3517	0.50	1/4723 (0.0%)
All	All	0.40	0/14068	0.52	1/18892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	51	ASP	CB-CG-OD1	5.33	123.10	118.30

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	3462	0	3467	21	0
1	B	3462	0	3467	28	0
1	C	3462	0	3467	20	0
1	D	3462	0	3467	15	0
2	A	28	0	42	5	0
2	B	24	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	42	1	0
2	D	8	0	12	2	0
3	A	186	0	0	1	0
3	B	121	0	0	0	0
3	C	176	0	0	2	0
3	D	139	0	0	1	0
All	All	14558	0	14000	84	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 (84) 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:105:SER:HB3	1:C:163:LYS:HD3	1.54	0.87
1:D:132:GLU:OE2	1:D:135:LYS:NZ	2.14	0.80
1:B:339:ILE:HD12	1:B:363:THR:HG22	1.70	0.73
1:A:354:ARG:NH1	3:A:601:HOH:O	2.22	0.71
1:B:61:ARG:HG2	1:B:421:LEU:HD11	1.74	0.69
1:A:412:ARG:HH22	2:A:507:EDO:H22	1.58	0.69
1:B:57:GLU:OE2	1:B:61:ARG:NH1	2.29	0.66
1:C:165:GLU:O	1:C:199:LYS:NZ	2.28	0.65
1:A:360:PRO:HA	2:A:505:EDO:H21	1.78	0.64
1:C:157:ASN:ND2	3:C:602:HOH:O	2.33	0.61
1:B:382:GLN:NE2	1:B:386:GLU:OE2	2.34	0.60
1:B:270:GLU:O	1:B:323:LYS:HE2	2.02	0.60
1:B:152:SER:OG	1:B:158:GLU:OE1	2.20	0.59
1:C:43:GLN:HG3	1:C:82:PHE:CD2	2.39	0.57
1:B:19:TYR:HB3	1:B:194:VAL:HG11	1.88	0.55
1:C:330:ASN:HB3	2:C:503:EDO:H12	1.88	0.55
1:B:101:PHE:CE2	1:B:190:THR:HG22	2.42	0.54
1:C:61:ARG:HG3	1:C:421:LEU:HD21	1.89	0.54
1:D:148:MET:HA	1:D:161:VAL:HG21	1.90	0.53
1:C:168:ASN:OD1	1:C:193:ARG:NH1	2.42	0.53
1:D:110:PHE:CE1	1:D:160:GLU:HG2	2.43	0.53
1:A:206:ARG:HB2	1:A:207:PHE:HD1	1.74	0.52
1:B:51:ASP:OD2	1:B:412:ARG:NH1	2.44	0.51
1:C:15:ASN:HD22	1:C:206:ARG:HG3	1.75	0.51
1:B:43:GLN:HG3	1:B:82:PHE:CD2	2.46	0.50
1:B:257:LEU:HD23	1:B:318:VAL:HG11	1.95	0.49
1:D:279:LEU:HD13	1:D:313:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLU:HB3	1:D:142:ALA:HA	1.95	0.49
1:B:166:LYS:O	1:B:170:ILE:HG13	2.12	0.49
1:C:193:ARG:HH21	1:C:196:ALA:HB3	1.77	0.49
1:B:289:GLN:HG2	3:D:725:HOH:O	2.12	0.48
1:C:221:ARG:HD2	1:C:224:GLU:OE2	2.14	0.48
1:A:1:MET:HB2	1:A:31:ASP:OD1	2.14	0.48
1:A:104:GLU:OE1	1:A:168:ASN:HB2	2.13	0.48
1:D:270:GLU:O	1:D:323:LYS:HE2	2.14	0.48
1:B:128:PHE:O	1:B:132:GLU:HG2	2.14	0.48
1:A:168:ASN:OD1	1:A:193:ARG:HD2	2.13	0.47
1:D:114:VAL:HG11	1:D:164:LEU:HD11	1.97	0.47
1:B:132:GLU:O	1:B:137:TYR:HB2	2.15	0.47
1:C:221:ARG:NH1	1:C:224:GLU:OE1	2.48	0.47
1:C:372:LEU:HD11	1:C:381:LYS:HG2	1.98	0.46
1:B:57:GLU:O	1:B:61:ARG:HG3	2.17	0.45
1:C:160:GLU:HA	1:C:163:LYS:HE3	1.98	0.45
1:A:206:ARG:HB2	1:A:207:PHE:CD1	2.51	0.45
1:D:20:HIS:ND1	1:D:191:ILE:HD11	2.32	0.45
1:B:221:ARG:NH1	1:B:224:GLU:OE1	2.49	0.44
1:A:144:LYS:HG2	1:A:148:MET:HE3	1.99	0.44
1:C:157:ASN:OD1	1:C:160:GLU:HG3	2.17	0.44
1:C:336:TYR:HB3	1:C:384:PHE:CE2	2.52	0.44
1:D:370:LYS:NZ	2:D:502:EDO:H11	2.33	0.44
1:A:206:ARG:HD2	1:A:207:PHE:CE1	2.53	0.44
1:A:332:LYS:O	2:A:501:EDO:H21	2.18	0.44
1:D:104:GLU:HG2	1:D:166:LYS:HD2	1.99	0.44
1:B:336:TYR:HB3	1:B:384:PHE:CE2	2.53	0.44
1:B:76:THR:O	1:B:312:ARG:HD2	2.18	0.44
1:A:279:LEU:HD13	1:A:313:LEU:CD1	2.48	0.44
1:D:43:GLN:HG3	1:D:82:PHE:CD2	2.53	0.44
1:A:40:ASN:HB3	1:A:398:TYR:CD2	2.53	0.43
1:B:8:VAL:O	1:B:37:MET:HA	2.19	0.43
1:C:15:ASN:ND2	1:C:206:ARG:HG3	2.34	0.43
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.81	0.42
1:D:144:LYS:HE2	1:D:144:LYS:HB3	1.89	0.42
1:B:193:ARG:NH1	1:B:195:GLY:O	2.44	0.42
1:A:279:LEU:HD13	1:A:313:LEU:HD11	2.00	0.42
1:C:405:VAL:HA	1:C:408:ARG:HD2	2.02	0.42
1:B:36:VAL:HG22	1:B:70:LEU:HB2	2.02	0.41
1:A:369:ARG:H	2:A:503:EDO:H12	1.85	0.41
1:B:221:ARG:HD2	1:B:224:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:VAL:O	1:C:37:MET:HA	2.21	0.41
1:D:171:LEU:HA	1:D:171:LEU:HD12	1.86	0.41
1:A:206:ARG:HA	1:A:207:PHE:HA	1.78	0.41
1:D:206:ARG:HG2	1:D:227:ASP:O	2.20	0.41
1:A:104:GLU:CD	1:A:166:LYS:HB3	2.41	0.41
1:A:221:ARG:HB3	1:A:224:GLU:OE2	2.21	0.41
1:A:328:LYS:HB3	1:A:328:LYS:HE2	1.92	0.41
1:D:122:PRO:HB2	1:D:124:GLU:OE1	2.21	0.41
1:A:369:ARG:HG3	2:A:503:EDO:H12	2.03	0.41
1:B:285:VAL:CG1	2:D:502:EDO:H12	2.51	0.41
1:B:105:SER:HB3	1:B:163:LYS:HD3	2.04	0.40
1:C:221:ARG:HB3	3:C:607:HOH:O	2.20	0.40
1:A:144:LYS:O	1:A:148:MET:HG3	2.21	0.40
1:B:124:GLU:HG2	1:B:153:MET:SD	2.61	0.40
1:C:193:ARG:NH2	1:C:196:ALA:HB3	2.36	0.40
1:B:60:LEU:HD22	1:B:343:THR:HG23	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	419/425 (99%)	414 (99%)	5 (1%)	0	100	100
1	B	419/425 (99%)	412 (98%)	7 (2%)	0	100	100
1	C	419/425 (99%)	414 (99%)	5 (1%)	0	100	100
1	D	419/425 (99%)	412 (98%)	7 (2%)	0	100	100
All	All	1676/1700 (99%)	1652 (99%)	24 (1%)	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	372/374 (100%)	370 (100%)	2 (0%)	88	92
1	B	372/374 (100%)	366 (98%)	6 (2%)	62	69
1	C	372/374 (100%)	369 (99%)	3 (1%)	81	86
1	D	372/374 (100%)	368 (99%)	4 (1%)	73	79
All	All	1488/1496 (100%)	1473 (99%)	15 (1%)	76	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	204	ARG
1	B	43	GLN
1	B	201	THR
1	B	226	ARG
1	B	313	LEU
1	B	368	TYR
1	B	421	LEU
1	C	208	SER
1	C	265	ASN
1	C	368	TYR
1	D	43	GLN
1	D	44	ARG
1	D	151	PHE
1	D	368	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	CSD	C	42	1	3,7,8	0.82	0	1,8,10	0.40	0
1	CME	D	409	1	8,9,10	0.95	1 (12%)	5,9,11	0.67	0
1	CSD	B	42	1	3,7,8	0.96	0	1,8,10	1.16	0
1	CSD	D	42	1	3,7,8	0.90	0	1,8,10	0.05	0
1	CME	B	409	1	8,9,10	1.09	1 (12%)	5,9,11	0.92	0
1	CME	A	409	1	8,9,10	0.96	0	5,9,11	0.73	0
1	CME	C	409	1	8,9,10	0.99	1 (12%)	5,9,11	0.93	0
1	CSD	A	42	1	3,7,8	0.76	0	1,8,10	0.13	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
1	CSD	C	42	1	-	1/2/6/8	-
1	CME	D	409	1	-	0/5/8/10	-
1	CSD	B	42	1	-	1/2/6/8	-
1	CSD	D	42	1	-	1/2/6/8	-
1	CME	B	409	1	-	2/5/8/10	-
1	CME	A	409	1	-	0/5/8/10	-
1	CME	C	409	1	-	0/5/8/10	-
1	CSD	A	42	1	-	1/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	CME	CB-SG	-2.39	1.73	1.81
1	C	409	CME	CB-SG	-2.05	1.75	1.81
1	D	409	CME	CB-SG	-2.02	1.75	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	42	CSD	CA-CB-SG-OD1
1	B	42	CSD	CA-CB-SG-OD1
1	D	42	CSD	CA-CB-SG-OD1
1	A	42	CSD	CA-CB-SG-OD1
1	B	409	CME	CE-SD-SG-CB
1	B	409	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	EDO	A	501	-	3,3,3	0.41	0	2,2,2	0.19	0
2	EDO	C	506	-	3,3,3	0.55	0	2,2,2	0.23	0
2	EDO	C	502	-	3,3,3	0.79	0	2,2,2	0.21	0
2	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.47	0
2	EDO	A	507	-	3,3,3	0.54	0	2,2,2	0.15	0
2	EDO	B	501	-	3,3,3	0.43	0	2,2,2	0.44	0
2	EDO	A	503	-	3,3,3	0.59	0	2,2,2	0.11	0
2	EDO	A	505	-	3,3,3	0.56	0	2,2,2	0.10	0
2	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	B	503	-	3,3,3	0.56	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	501	-	3,3,3	0.43	0	2,2,2	0.54	0
2	EDO	A	506	-	3,3,3	0.51	0	2,2,2	0.30	0
2	EDO	B	502	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.57	0
2	EDO	A	502	-	3,3,3	0.38	0	2,2,2	0.57	0
2	EDO	C	503	-	3,3,3	0.35	0	2,2,2	0.74	0
2	EDO	B	504	-	3,3,3	0.40	0	2,2,2	0.54	0
2	EDO	C	505	-	3,3,3	0.43	0	2,2,2	0.65	0
2	EDO	D	502	-	3,3,3	0.53	0	2,2,2	0.19	0
2	EDO	C	507	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	D	501	-	3,3,3	0.51	0	2,2,2	0.41	0
2	EDO	C	504	-	3,3,3	0.37	0	2,2,2	0.45	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	A	501	-	-	1/1/1/1	-
2	EDO	C	506	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	B	506	-	-	1/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
2	EDO	C	501	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	C	505	-	-	1/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	C	504	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	B	505	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	C	505	EDO	O1-C1-C2-O2
2	A	507	EDO	O1-C1-C2-O2
2	B	503	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	B	506	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	EDO	1	0
2	A	507	EDO	1	0
2	A	503	EDO	2	0
2	A	505	EDO	1	0
2	C	503	EDO	1	0
2	D	502	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, 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	421/425 (99%)	-0.18	6 (1%) 75 78	20, 32, 65, 120	0
1	B	421/425 (99%)	0.12	23 (5%) 25 31	25, 40, 88, 127	0
1	C	421/425 (99%)	-0.16	8 (1%) 66 71	22, 33, 65, 140	0
1	D	421/425 (99%)	0.61	63 (14%) 2 3	22, 41, 133, 174	0
All	All	1684/1700 (99%)	0.10	100 (5%) 22 27	20, 36, 96, 174	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	TRP	11.3
1	D	195	GLY	9.0
1	B	194	VAL	8.5
1	D	145	TYR	8.1
1	D	162	LEU	7.6
1	D	155	GLY	7.5
1	D	136	GLY	7.4
1	D	157	ASN	7.3
1	D	137	TYR	7.0
1	D	147	LEU	6.5
1	D	194	VAL	6.3
1	D	204	ARG	6.2
1	C	196	ALA	6.1
1	D	154	LYS	6.1
1	D	153	MET	5.8
1	D	151	PHE	5.6
1	D	130	HIS	5.5
1	D	196	ALA	5.3
1	D	193	ARG	5.2
1	B	133	LEU	5.0
1	D	138	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	140	PRO	4.9
1	D	152	SER	4.9
1	D	158	GLU	4.8
1	B	130	HIS	4.8
1	D	203	PHE	4.7
1	D	160	GLU	4.5
1	C	194	VAL	4.5
1	B	134	LYS	4.4
1	C	203	PHE	4.4
1	D	150	TYR	4.2
1	D	134	LYS	4.2
1	D	201	THR	4.2
1	D	133	LEU	4.2
1	B	156	TRP	4.2
1	D	125	TYR	4.1
1	C	195	GLY	4.1
1	D	126	GLN	4.1
1	D	163	LYS	4.1
1	A	206	ARG	4.1
1	B	135	LYS	4.0
1	C	206	ARG	4.0
1	D	159	GLU	3.9
1	D	197	GLU	3.9
1	B	206	ARG	3.9
1	B	127	LYS	3.9
1	D	116	ARG	3.8
1	D	202	SER	3.7
1	D	168	ASN	3.7
1	D	127	LYS	3.6
1	B	137	TYR	3.5
1	A	202	SER	3.5
1	B	139	PHE	3.5
1	D	207	PHE	3.3
1	D	108	ILE	3.3
1	D	161	VAL	3.3
1	D	200	ASP	3.2
1	C	204	ARG	3.2
1	D	128	PHE	3.2
1	B	123	ASP	3.2
1	D	107	ASP	3.2
1	B	136	GLY	3.1
1	D	303	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	141	ASN	3.1
1	D	139	PHE	3.0
1	B	151	PHE	3.0
1	D	205	GLY	2.9
1	A	205	GLY	2.9
1	B	205	GLY	2.9
1	B	141	ASN	2.9
1	D	122	PRO	2.9
1	B	162	LEU	2.9
1	D	164	LEU	2.9
1	B	163	LYS	2.9
1	D	192	LYS	2.8
1	B	122	PRO	2.8
1	C	207	PHE	2.7
1	D	135	LYS	2.7
1	D	121	GLN	2.6
1	B	207	PHE	2.6
1	D	117	ILE	2.6
1	D	165	GLU	2.6
1	D	206	ARG	2.6
1	A	201	THR	2.4
1	D	120	GLU	2.3
1	D	166	LYS	2.3
1	D	148	MET	2.3
1	A	197	GLU	2.3
1	B	153	MET	2.3
1	D	146	ALA	2.2
1	B	19	TYR	2.2
1	D	123	ASP	2.2
1	C	201	THR	2.2
1	D	106	ASN	2.2
1	D	129	LEU	2.2
1	A	198	GLU	2.2
1	B	126	GLN	2.1
1	D	149	ARG	2.1
1	B	138	SER	2.1
1	D	105	SER	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, 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	B-factors(Å ²)	Q<0.9
1	CME	B	409	10/11	0.92	0.14	38,46,91,92	0
1	CME	C	409	10/11	0.94	0.12	22,32,79,98	0
1	CSD	C	42	8/9	0.95	0.11	24,25,41,91	0
1	CSD	B	42	8/9	0.95	0.13	25,32,51,83	0
1	CME	A	409	10/11	0.97	0.13	22,33,48,48	0
1	CSD	D	42	8/9	0.97	0.11	31,34,47,61	0
1	CSD	A	42	8/9	0.97	0.08	23,29,53,62	0
1	CME	D	409	10/11	0.98	0.12	25,32,39,47	0

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, 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	B-factors(Å ²)	Q<0.9
2	EDO	A	503	4/4	0.40	0.38	63,65,65,67	0
2	EDO	C	506	4/4	0.51	0.34	70,74,74,74	0
2	EDO	D	502	4/4	0.63	0.29	53,61,65,66	0
2	EDO	D	501	4/4	0.69	0.25	53,54,55,55	0
2	EDO	B	503	4/4	0.76	0.27	42,55,56,62	0
2	EDO	A	505	4/4	0.78	0.19	42,51,54,57	0
2	EDO	A	507	4/4	0.81	0.35	58,60,64,64	0
2	EDO	C	501	4/4	0.81	0.21	61,63,64,65	0
2	EDO	B	506	4/4	0.83	0.32	55,58,65,70	0
2	EDO	A	506	4/4	0.84	0.13	58,60,60,64	0
2	EDO	C	502	4/4	0.86	0.14	29,29,30,33	0
2	EDO	B	501	4/4	0.86	0.22	41,46,58,58	0
2	EDO	C	503	4/4	0.91	0.20	57,61,61,62	0
2	EDO	C	505	4/4	0.91	0.30	49,50,54,57	0
2	EDO	A	504	4/4	0.92	0.20	46,55,61,67	0
2	EDO	C	507	4/4	0.93	0.23	42,43,56,60	0
2	EDO	A	502	4/4	0.93	0.21	50,52,54,64	0
2	EDO	B	502	4/4	0.94	0.16	28,35,41,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	505	4/4	0.94	0.15	50,51,55,58	0
2	EDO	A	501	4/4	0.98	0.16	34,35,36,37	0
2	EDO	B	504	4/4	0.98	0.15	28,30,36,37	0
2	EDO	C	504	4/4	0.99	0.16	27,28,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.