



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:41 PM UTC

PDB ID : 5Y0S / pdb_00005y0s
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

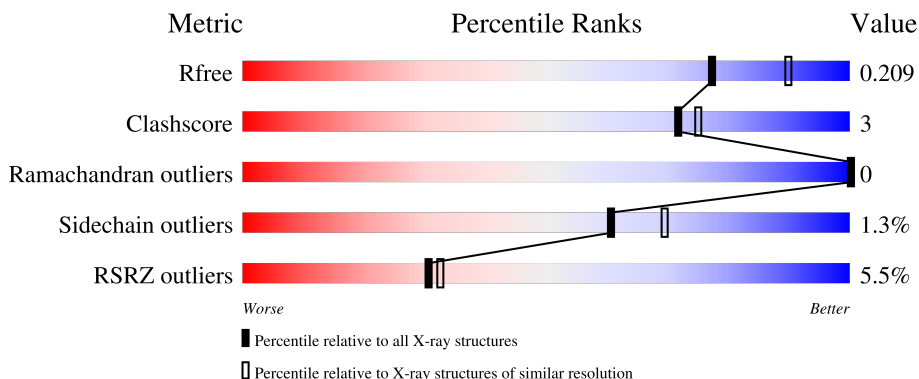
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	0% 93% 7%
1	B	425	6% 87% 12%
1	C	425	3% 90% 9%
1	D	425	11% 92% 7%

2 Entry composition [i](#)

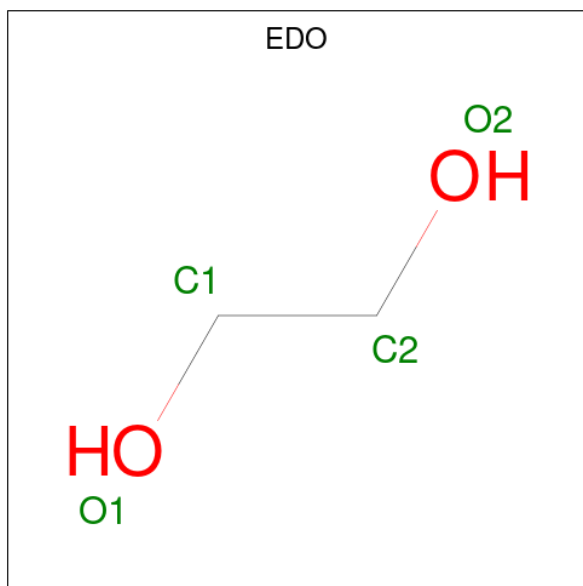
There are 3 unique types of molecules in this entry. The entry contains 14558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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

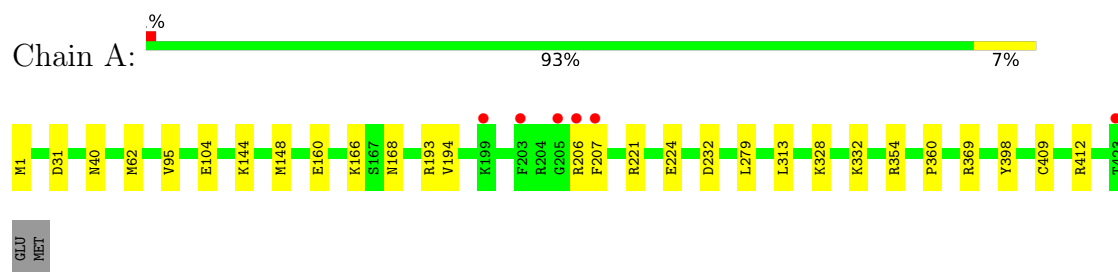
- Molecule 3 is water.

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

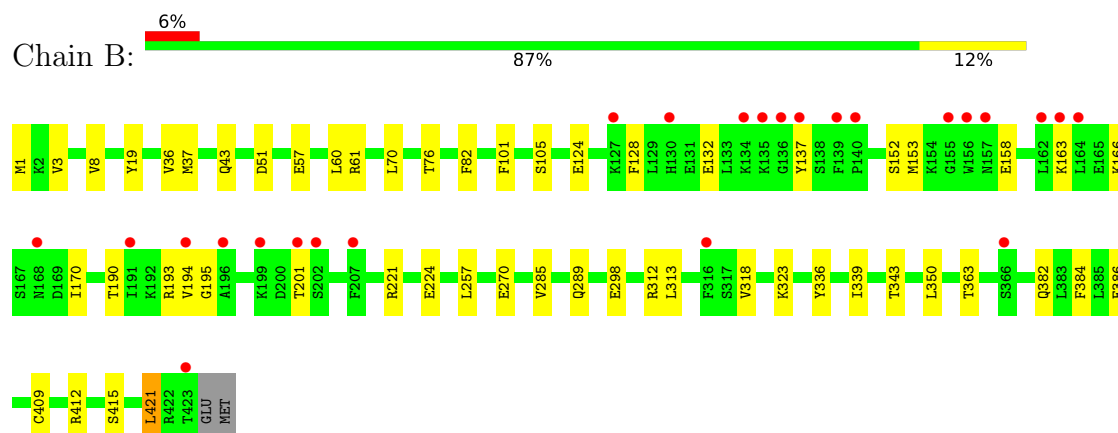
3 Residue-property plots

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.

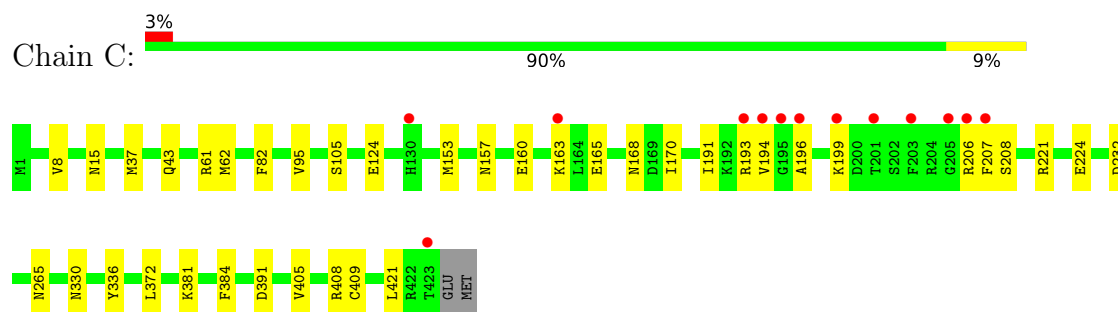
• Molecule 1: *Thermotoga maritima* TmcAL



• Molecule 1: *Thermotoga maritima* TmcAL

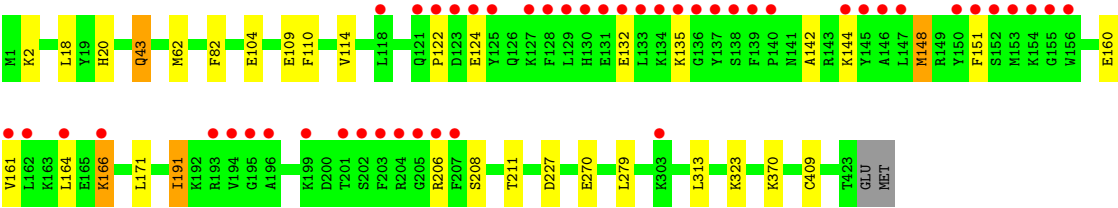


• Molecule 1: *Thermotoga maritima* TmcAL



• 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	80.99Å 97.95Å 144.28Å 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 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.169 , 0.207 0.172 , 0.209	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 , 44.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, CSD, 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	0.53	0/3517	0.75	1/4723 (0.0%)
1	B	0.46	0/3517	0.74	0/4723
1	C	0.52	0/3517	0.77	3/4723 (0.1%)
1	D	0.48	0/3517	0.74	0/4723
All	All	0.50	0/14068	0.75	4/18892 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	VAL	N-CA-C	-6.82	103.72	113.07
1	A	95	VAL	N-CA-C	5.84	119.36	113.47
1	C	207	PHE	N-CA-C	5.44	118.92	112.72
1	C	95	VAL	N-CA-C	5.14	119.03	113.43

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	3462	0	3467	22	0
1	B	3462	0	3467	30	0
1	C	3462	0	3467	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3462	0	3467	17	0
2	A	28	0	42	5	0
2	B	24	0	36	0	0
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	93	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 (93) 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:B:339:ILE:HD12	1:B:363:THR:HG22	1.70	0.73
1:D:132:GLU:OE2	1:D:135:LYS:NZ	2.14	0.71
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:A:144:LYS:HG2	1:A:148:MET:HE3	1.75	0.66
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:C:336:TYR:OH	1:C:391:ASP:OD2	2.20	0.52
1:A:206:ARG:HB2	1:A:207:PHE:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:MET:HE3	1:C:232:ASP:HB2	1.92	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
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:62:MET:HA	1:C:62:MET:HE2	1.95	0.48
1:C:221:ARG:HD2	1:C:224:GLU:OE2	2.14	0.48
1:D:104:GLU:HB3	1:D:166:LYS:HZ3	1.77	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:A:104:GLU:CD	1:A:166:LYS:HB3	2.41	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: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:76:THR:O	1:B:312:ARG:HD2	2.18	0.44
1:B:336:TYR:HB3	1:B:384:PHE:CE2	2.53	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:A:62:MET:HE3	1:A:232:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:GLU:HG2	1:C:153:MET:HE1	2.01	0.42
1:C:405:VAL:HA	1:C:408:ARG:HD2	2.02	0.42
1:B:412:ARG:HA	1:B:415:SER:HG	1.84	0.42
1:B:1:MET:HE3	1:B:3:VAL:HG23	2.02	0.41
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
1:C:8:VAL:O	1:C:37:MET:HA	2.21	0.41
1:D:171:LEU:HD12	1:D:171:LEU:HA	1.86	0.41
1:D:18:LEU:HD13	1:D:62:MET:HE3	2.01	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:221:ARG:HB3	1:A:224:GLU:OE2	2.21	0.41
1:A:328:LYS:HE2	1:A:328:LYS:HB3	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 [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	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%)	81	88
1	B	372/374 (100%)	368 (99%)	4 (1%)	65	74
1	C	372/374 (100%)	368 (99%)	4 (1%)	65	74
1	D	372/374 (100%)	363 (98%)	9 (2%)	43	49
All	All	1488/1496 (100%)	1469 (99%)	19 (1%)	61	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	A	194	VAL
1	B	201	THR
1	B	298	GLU
1	B	313	LEU
1	B	421	LEU
1	C	170	ILE
1	C	191	ILE
1	C	208	SER
1	C	265	ASN
1	D	2	LYS
1	D	43	GLN
1	D	109	GLU

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Mol	Chain	Res	Type
1	D	148	MET
1	D	151	PHE
1	D	166	LYS
1	D	191	ILE
1	D	208	SER
1	D	211	THR

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

Mol	Chain	Res	Type
1	A	130	HIS
1	A	382	GLN
1	C	121	GLN

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	CME	B	409	1	8,9,10	1.09	1 (12%)	6,9,11	2.02	1 (16%)
1	CSD	D	42	1	4,7,8	1.13	0	1,8,10	0.02	0
1	CME	C	409	1	8,9,10	1.00	1 (12%)	6,9,11	1.86	1 (16%)
1	CSD	A	42	1	4,7,8	1.00	0	1,8,10	0.10	0
1	CSD	B	42	1	4,7,8	0.98	0	1,8,10	1.24	0
1	CME	D	409	1	8,9,10	0.95	0	6,9,11	1.47	1 (16%)
1	CME	A	409	1	8,9,10	0.97	0	6,9,11	1.09	1 (16%)
1	CSD	C	42	1	4,7,8	0.83	0	1,8,10	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
1	CME	B	409	1	-	2/5/8/10	-
1	CSD	D	42	1	-	1/2/6/8	-
1	CME	C	409	1	-	0/5/8/10	-
1	CSD	A	42	1	-	1/2/6/8	-
1	CSD	B	42	1	-	1/2/6/8	-
1	CME	D	409	1	-	0/5/8/10	-
1	CME	A	409	1	-	0/5/8/10	-
1	CSD	C	42	1	-	1/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	CME	CB-SG	-2.34	1.73	1.81
1	C	409	CME	CB-SG	-2.02	1.75	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	CME	CB-CA-C	-4.50	98.58	110.80
1	C	409	CME	CB-CA-C	-4.06	99.76	110.80
1	D	409	CME	CB-CA-C	-3.28	101.89	110.80
1	A	409	CME	CB-CA-C	-2.10	105.10	110.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	42	CSD	CA-CB-SG-OD1
1	B	42	CSD	CA-CB-SG-OD1
1	C	42	CSD	CA-CB-SG-OD1
1	D	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	504	-	3,3,3	0.34	0	2,2,2	0.48	0
2	EDO	A	502	-	3,3,3	0.36	0	2,2,2	0.60	0
2	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.13	0
2	EDO	D	501	-	3,3,3	0.48	0	2,2,2	0.45	0
2	EDO	B	504	-	3,3,3	0.37	0	2,2,2	0.57	0
2	EDO	A	504	-	3,3,3	0.37	0	2,2,2	0.60	0
2	EDO	A	501	-	3,3,3	0.38	0	2,2,2	0.24	0
2	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	A	507	-	3,3,3	0.51	0	2,2,2	0.20	0
2	EDO	C	507	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	C	506	-	3,3,3	0.52	0	2,2,2	0.28	0
2	EDO	B	505	-	3,3,3	0.41	0	2,2,2	0.51	0
2	EDO	C	503	-	3,3,3	0.32	0	2,2,2	0.76	0
2	EDO	C	505	-	3,3,3	0.40	0	2,2,2	0.67	0
2	EDO	C	502	-	3,3,3	0.77	0	2,2,2	0.14	0
2	EDO	B	506	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	B	503	-	3,3,3	0.53	0	2,2,2	0.26	0
2	EDO	A	503	-	3,3,3	0.56	0	2,2,2	0.17	0
2	EDO	B	501	-	3,3,3	0.40	0	2,2,2	0.48	0
2	EDO	D	502	-	3,3,3	0.50	0	2,2,2	0.22	0
2	EDO	B	502	-	3,3,3	0.62	0	2,2,2	0.11	0
2	EDO	C	501	-	3,3,3	0.41	0	2,2,2	0.57	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	C	504	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	C	506	-	-	0/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	C	505	-	-	1/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	B	506	-	-	1/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	C	501	-	-	1/1/1/1	-

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	B	505	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	A	507	EDO	O1-C1-C2-O2
2	B	503	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	C	505	EDO	O1-C1-C2-O2
2	B	502	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	505	EDO	1	0
2	A	501	EDO	1	0
2	A	507	EDO	1	0
2	C	503	EDO	1	0
2	A	503	EDO	2	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%)	-0.31	6 (1%) 73 75	20, 32, 65, 120	0
1	B	421/425 (99%)	0.05	25 (5%) 28 30	25, 40, 88, 127	0
1	C	421/425 (99%)	-0.26	13 (3%) 51 54	22, 33, 65, 140	0
1	D	421/425 (99%)	0.21	48 (11%) 10 10	22, 41, 133, 174	0
All	All	1684/1700 (99%)	-0.08	92 (5%) 30 32	20, 36, 96, 174	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	194	VAL	7.5
1	B	194	VAL	6.1
1	C	196	ALA	6.1
1	D	194	VAL	5.6
1	B	162	LEU	5.5
1	B	201	THR	5.1
1	C	195	GLY	4.9
1	D	134	LYS	4.8
1	B	163	LYS	4.8
1	D	133	LEU	4.7
1	C	201	THR	4.6
1	D	195	GLY	4.5
1	D	156	TRP	4.2
1	D	201	THR	4.2
1	D	130	HIS	4.2
1	A	206	ARG	4.1
1	C	203	PHE	4.1
1	B	423	THR	4.1
1	D	196	ALA	3.9
1	C	199	LYS	3.8
1	D	205	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	151	PHE	3.8
1	D	127	LYS	3.8
1	D	139	PHE	3.7
1	B	199	LYS	3.5
1	D	202	SER	3.4
1	D	164	LEU	3.3
1	D	140	PRO	3.3
1	B	134	LYS	3.3
1	D	128	PHE	3.3
1	D	135	LYS	3.3
1	D	125	TYR	3.2
1	D	203	PHE	3.2
1	C	205	GLY	3.2
1	D	147	LEU	3.2
1	D	145	TYR	3.1
1	B	168	ASN	3.1
1	A	205	GLY	3.0
1	B	135	LYS	3.0
1	D	150	TYR	2.9
1	B	139	PHE	2.9
1	D	161	VAL	2.9
1	B	156	TRP	2.9
1	D	129	LEU	2.8
1	D	162	LEU	2.8
1	D	138	SER	2.8
1	C	163	LYS	2.8
1	D	199	LYS	2.7
1	C	193	ARG	2.7
1	D	137	TYR	2.7
1	D	153	MET	2.7
1	C	130	HIS	2.6
1	D	123	ASP	2.6
1	D	131	GLU	2.6
1	A	199	LYS	2.6
1	B	155	GLY	2.5
1	D	166	LYS	2.5
1	B	164	LEU	2.5
1	B	130	HIS	2.5
1	C	423	THR	2.5
1	D	155	GLY	2.4
1	A	423	THR	2.4
1	D	136	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	124	GLU	2.3
1	D	204	ARG	2.3
1	D	144	LYS	2.3
1	D	118	LEU	2.3
1	B	202	SER	2.2
1	D	121	GLN	2.2
1	D	152	SER	2.2
1	A	207	PHE	2.2
1	B	127	LYS	2.2
1	B	140	PRO	2.2
1	B	137	TYR	2.2
1	A	203	PHE	2.2
1	D	206	ARG	2.1
1	B	207	PHE	2.1
1	B	136	GLY	2.1
1	C	206	ARG	2.1
1	D	154	LYS	2.1
1	D	132	GLU	2.1
1	D	207	PHE	2.1
1	D	193	ARG	2.1
1	B	191	ILE	2.1
1	D	303	LYS	2.1
1	B	196	ALA	2.1
1	D	146	ALA	2.1
1	B	157	ASN	2.0
1	D	122	PRO	2.0
1	B	316	PHE	2.0
1	C	207	PHE	2.0
1	B	366	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($\text{\AA}^2$)	Q<0.9
1	CME	B	409	10/11	0.89	0.14	38,46,91,92	0
1	CME	C	409	10/11	0.92	0.14	22,32,79,98	0
1	CSD	B	42	8/9	0.96	0.08	25,32,51,83	0
1	CSD	C	42	8/9	0.97	0.09	24,25,41,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSD	A	42	8/9	0.97	0.06	23,29,53,62	0
1	CSD	D	42	8/9	0.97	0.07	31,34,47,61	0
1	CME	D	409	10/11	0.97	0.08	25,32,39,47	0
1	CME	A	409	10/11	0.98	0.06	22,33,48,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EDO	D	501	4/4	0.75	0.21	53,54,55,55	0
2	EDO	A	503	4/4	0.77	0.23	63,65,65,67	0
2	EDO	C	506	4/4	0.78	0.24	70,74,74,74	0
2	EDO	D	502	4/4	0.79	0.20	53,61,65,66	0
2	EDO	B	503	4/4	0.82	0.19	42,55,56,62	0
2	EDO	A	507	4/4	0.82	0.22	58,60,64,64	0
2	EDO	C	501	4/4	0.85	0.19	61,63,64,65	0
2	EDO	B	506	4/4	0.86	0.18	55,58,65,70	0
2	EDO	A	505	4/4	0.87	0.16	42,51,54,57	0
2	EDO	C	507	4/4	0.88	0.14	42,43,56,60	0
2	EDO	A	506	4/4	0.88	0.15	58,60,60,64	0
2	EDO	A	502	4/4	0.88	0.16	50,52,54,64	0
2	EDO	B	505	4/4	0.90	0.10	50,51,55,58	0
2	EDO	C	502	4/4	0.90	0.14	29,29,30,33	0
2	EDO	B	501	4/4	0.90	0.18	41,46,58,58	0
2	EDO	A	504	4/4	0.91	0.16	46,55,61,67	0
2	EDO	C	505	4/4	0.91	0.16	49,50,54,57	0
2	EDO	C	503	4/4	0.92	0.17	57,61,61,62	0
2	EDO	B	502	4/4	0.95	0.11	28,35,41,43	0
2	EDO	C	504	4/4	0.96	0.07	27,28,30,30	0
2	EDO	B	504	4/4	0.96	0.07	28,30,36,37	0
2	EDO	A	501	4/4	0.97	0.07	34,35,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.