Full wwPDB X-ray Structure Validation Report (i)

Nov 9, 2024 – 11:07 pm GMT

PDB ID	:	6TMM
Title	:	BIL2 domain from T.thermophila BUBL1 locus (C1A-N143A)
Authors	:	Chiarini, V.; Ilari, A.
Deposited on	:	2019-12-04
Resolution	:	2.40 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.40 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		4.3%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
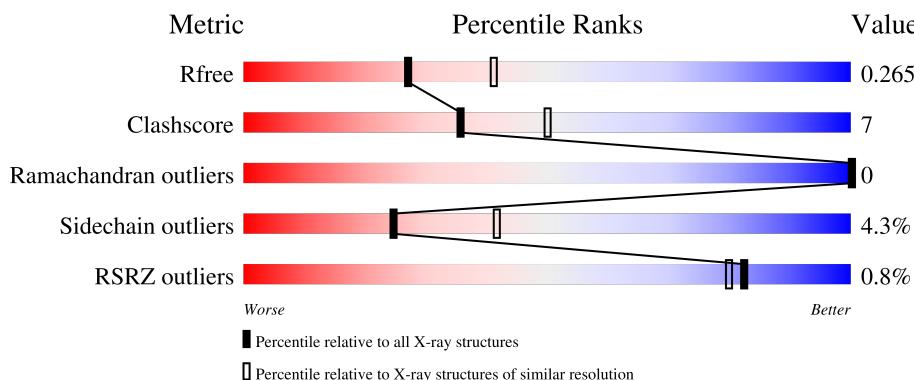
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	AAA	156	85% 14% ·
1	CCC	156	90% 8% ·
2	BBB	155	90% 9% ·
2	DDD	155	86% 12% ·
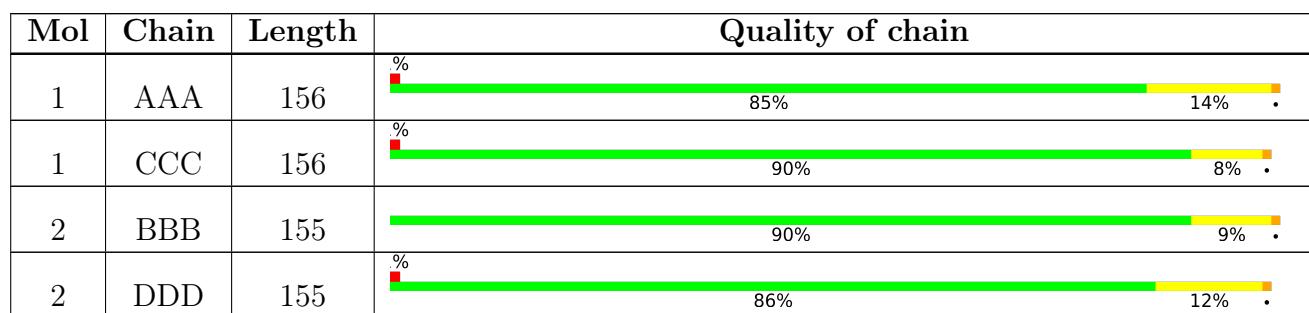
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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
4	PEG	AAA	804	-	-	X	-

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 5204 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 NAD(P)(+)–arginine ADP-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	156	Total 1269	C 809	N 217	O 238	S 5	0	2	0
1	CCC	156	Total 1256	C 802	N 214	O 235	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	ALA	CYS	engineered mutation	UNP Q236S9
AAA	143	ALA	ASN	engineered mutation	UNP Q236S9
CCC	1	ALA	CYS	engineered mutation	UNP Q236S9
CCC	143	ALA	ASN	engineered mutation	UNP Q236S9

- Molecule 2 is a protein called NAD(P)(+)–arginine ADP-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	155	Total 1263	C 803	N 216	O 239	S 5	0	2	0
2	DDD	155	Total 1248	C 796	N 213	O 234	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	1	ALA	CYS	engineered mutation	UNP Q236S9
BBB	143	ALA	ASN	engineered mutation	UNP Q236S9
DDD	1	ALA	CYS	engineered mutation	UNP Q236S9
DDD	143	ALA	ASN	engineered mutation	UNP Q236S9

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

FMT

C

OH O2

O

O1
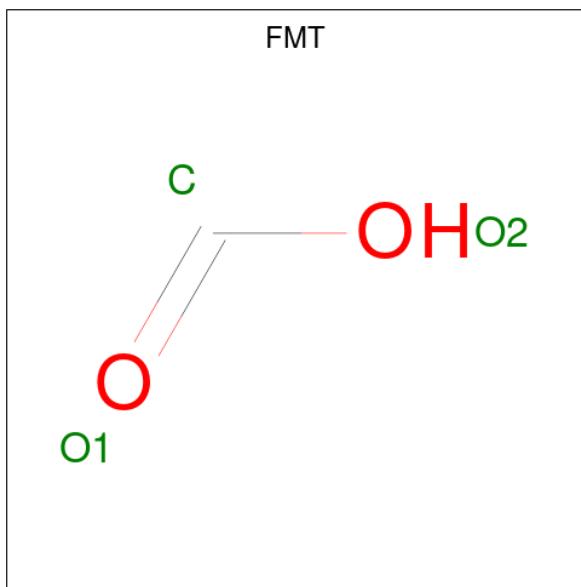
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total 3	C 1	O 2	0	0
3	AAA	1	Total 3	C 1	O 2	0	0
3	AAA	1	Total 3	C 1	O 2	0	0
3	AAA	1	Total 3	C 1	O 2	0	0
3	BBB	1	Total 3	C 1	O 2	0	0
3	BBB	1	Total 3	C 1	O 2	0	0
3	BBB	1	Total 3	C 1	O 2	0	0
3	CCC	1	Total 3	C 1	O 2	0	0
3	CCC	1	Total 3	C 1	O 2	0	0
3	DDD	1	Total 3	C 1	O 2	0	0
3	DDD	1	Total 3	C 1	O 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
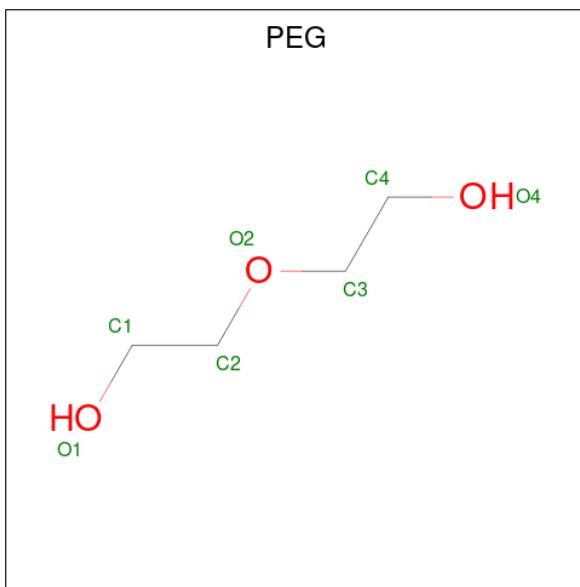
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total 7	C 4	O 3	0	0

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total 1	Hg 1	0	0
5	BBB	1	Total 1	Hg 1	0	0
5	CCC	1	Total 1	Hg 1	0	0
5	DDD	1	Total 1	Hg 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	1	Total 1	Ca 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	33	Total 33	O 33	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	BBB	25	Total 25	O 25	0	0
7	CCC	40	Total 40	O 40	0	0
7	DDD	25	Total 25	O 25	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: NAD(P)(+)–arginine ADP-ribosyltransferase
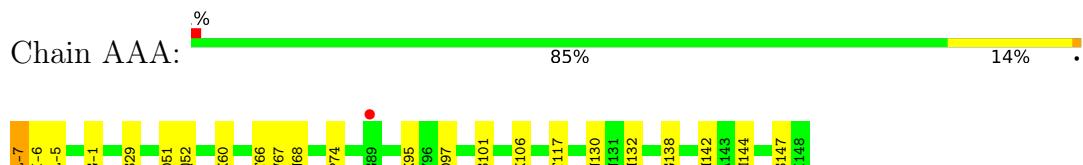
Chain AAA:

• Molecule 1: NAD(P)(+)–arginine ADP-ribosyltransferase

Chain CCC:

• Molecule 2: NAD(P)(+)–arginine ADP-ribosyltransferase

Chain BBB:

• Molecule 2: NAD(P)(+)–arginine ADP-ribosyltransferase

Chain DDD:
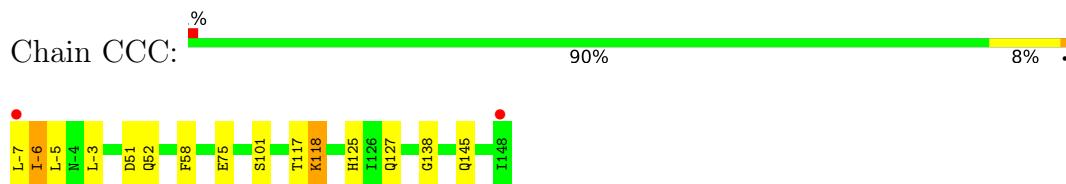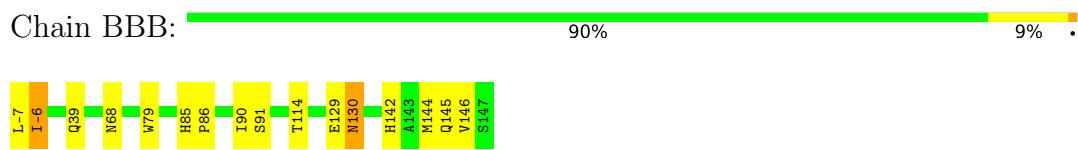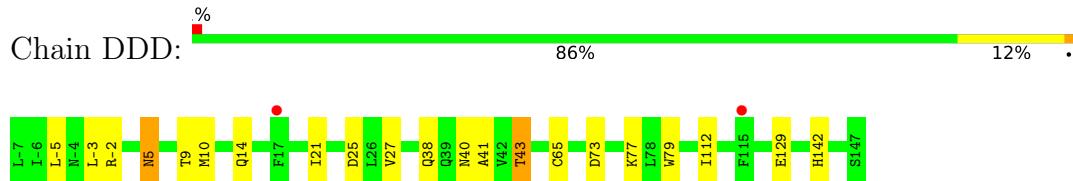
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.48Å 72.77Å 70.26Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	69.60 – 2.40 69.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.60-2.40) 99.4 (69.60-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.198 , 0.267 0.204 , 0.265	Depositor DCC
R_{free} test set	1346 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.5	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5204	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FMT, CA, PEG, HG

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	AAA	0.62	0/1299	0.76	0/1756
1	CCC	0.63	0/1283	0.75	0/1734
2	BBB	0.65	0/1290	0.74	0/1742
2	DDD	0.64	0/1275	0.74	0/1723
All	All	0.64	0/5147	0.75	0/6955

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 ⓘ

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	AAA	1269	0	1252	33	0
1	CCC	1256	0	1241	9	0
2	BBB	1263	0	1240	17	0
2	DDD	1248	0	1231	16	0
3	AAA	12	0	4	1	0
3	BBB	9	0	3	0	0
3	CCC	6	0	2	1	0
3	DDD	6	0	2	1	0
4	AAA	7	0	10	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	1	0	0	0	0
7	AAA	33	0	0	4	0
7	BBB	25	0	0	2	0
7	CCC	40	0	0	1	0
7	DDD	25	0	0	7	0
All	All	5204	0	4985	72	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 7.

All (72) 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:AAA:52:GLN:CB	4:AAA:804:PEG:H42	1.68	1.23
1:AAA:52:GLN:HB2	4:AAA:804:PEG:C4	1.80	1.10
4:AAA:804:PEG:H12	2:BBB:86:PRO:CG	1.82	1.08
4:AAA:804:PEG:H12	2:BBB:86:PRO:HG3	1.13	1.06
1:AAA:52:GLN:HB2	4:AAA:804:PEG:H42	1.09	1.05
1:AAA:67:VAL:H	4:AAA:804:PEG:H22	1.11	1.05
1:AAA:67:VAL:H	4:AAA:804:PEG:C2	1.71	1.04
4:AAA:804:PEG:C1	2:BBB:86:PRO:HG3	2.00	0.90
4:AAA:804:PEG:H11	2:BBB:86:PRO:HD3	1.57	0.85
1:AAA:52:GLN:HB3	4:AAA:804:PEG:H42	1.60	0.82
4:AAA:804:PEG:C1	2:BBB:86:PRO:HD3	2.12	0.78
1:AAA:67:VAL:N	4:AAA:804:PEG:H22	1.94	0.78
2:DDD:-2:ARG:HA	3:DDD:602:FMT:C	2.15	0.77
1:AAA:66:THR:HA	4:AAA:804:PEG:H21	1.69	0.74
4:AAA:804:PEG:C1	2:BBB:86:PRO:CG	2.64	0.71
2:DDD:65:CYS:SG	7:DDD:717:HOH:O	2.47	0.71
1:AAA:66:THR:CA	4:AAA:804:PEG:H21	2.25	0.66
1:AAA:67:VAL:HG22	4:AAA:804:PEG:H22	1.77	0.65
2:DDD:40:ASN:O	7:DDD:701:HOH:O	2.14	0.64
4:AAA:804:PEG:C1	2:BBB:86:PRO:CD	2.74	0.64
4:AAA:804:PEG:H41	2:BBB:86:PRO:HA	1.82	0.62
2:DDD:5:ASN:HB2	7:DDD:712:HOH:O	2.00	0.60
1:AAA:67:VAL:N	4:AAA:804:PEG:C2	2.55	0.59
1:AAA:68[B]:ASN:OD1	4:AAA:804:PEG:O1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:130:ASN:N	7:AAA:901:HOH:O	2.12	0.58
4:AAA:804:PEG:H11	2:BBB:86:PRO:CD	2.32	0.56
2:DDD:25:ASP:O	7:DDD:701:HOH:O	2.18	0.56
1:AAA:68[B]:ASN:CG	4:AAA:804:PEG:O1	2.45	0.55
1:AAA:52:GLN:NE2	2:BBB:90:ILE:O	2.39	0.55
1:AAA:67:VAL:HG13	4:AAA:804:PEG:H22	1.89	0.55
2:BBB:68:ASN:HD21	2:BBB:85:HIS:CE1	2.24	0.54
1:AAA:67:VAL:H	4:AAA:804:PEG:H21	1.64	0.54
2:BBB:68:ASN:ND2	2:BBB:85:HIS:CE1	2.77	0.53
2:DDD:43:THR:HG22	2:DDD:129:GLU:HG3	1.90	0.52
2:DDD:112:ILE:HG23	7:DDD:721:HOH:O	2.10	0.51
1:AAA:52:GLN:HE22	2:BBB:91:SER:HA	1.76	0.50
1:AAA:66:THR:HB	4:AAA:804:PEG:H21	1.95	0.49
1:AAA:-5:LEU:HG	7:AAA:921:HOH:O	2.13	0.48
2:BBB:-6:ILE:HD11	1:CCC:-6:ILE:HD11	1.94	0.48
1:CCC:118:LYS:HE3	1:CCC:118:LYS:HA	1.95	0.48
2:DDD:73:ASP:O	2:DDD:77:LYS:N	2.47	0.48
2:DDD:10:MET:HA	2:DDD:27:VAL:HA	1.96	0.47
1:CCC:-3:LEU:HB3	1:CCC:125:HIS:CD2	2.51	0.46
1:CCC:51:ASP:HA	1:CCC:117:THR:HG22	1.97	0.46
1:AAA:66:THR:CB	4:AAA:804:PEG:H21	2.46	0.45
1:AAA:101:SER:HA	1:AAA:138:GLY:O	2.16	0.45
1:AAA:74:PRO:HG2	1:AAA:106:LYS:HG2	1.98	0.45
1:AAA:-6:ILE:HD13	7:AAA:924:HOH:O	2.16	0.45
1:CCC:101:SER:HA	1:CCC:138:GLY:O	2.18	0.44
1:AAA:97:ASP:OD1	3:AAA:803:FMT:C	2.66	0.44
1:AAA:-1:GLY:HA3	1:AAA:142:HIS:O	2.18	0.43
1:CCC:-6:ILE:HD13	1:CCC:-6:ILE:C	2.39	0.43
1:AAA:67:VAL:HG13	4:AAA:804:PEG:C2	2.48	0.43
1:CCC:52:GLN:HG2	7:CCC:701:HOH:O	2.17	0.43
1:AAA:-7:LEU:HB3	2:DDD:-3:LEU:HB2	2.01	0.43
1:AAA:67:VAL:CG2	4:AAA:804:PEG:H22	2.47	0.42
2:BBB:144:MET:HE2	7:BBB:514:HOH:O	2.19	0.42
2:DDD:41:ALA:HA	7:DDD:701:HOH:O	2.19	0.42
1:AAA:51:ASP:HA	1:AAA:117:THR:OG1	2.20	0.42
1:CCC:125:HIS:HA	3:CCC:601:FMT:C	2.49	0.42
1:AAA:67:VAL:N	4:AAA:804:PEG:H21	2.32	0.42
4:AAA:804:PEG:H11	4:AAA:804:PEG:H32	1.68	0.41
2:DDD:-3:LEU:N	2:DDD:-3:LEU:HD22	2.36	0.41
1:AAA:130:ASN:O	1:AAA:132:HIS:CE1	2.74	0.41
2:DDD:-5:LEU:HD23	2:DDD:-5:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:79:TRP:CH2	2:DDD:142:HIS:HB2	2.56	0.41
2:DDD:38:GLN:HE21	2:DDD:38:GLN:HB3	1.69	0.41
2:BBB:130[A]:ASN:ND2	7:BBB:504:HOH:O	2.55	0.40
2:BBB:79:TRP:CZ3	2:BBB:142:HIS:HB2	2.56	0.40
1:CCC:-5:LEU:HD21	1:CCC:145:GLN:HG3	2.02	0.40
1:AAA:95:LYS:HD2	7:AAA:922:HOH:O	2.22	0.40
2:DDD:112:ILE:CG2	7:DDD:721:HOH:O	2.69	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	AAA	156/156 (100%)	150 (96%)	6 (4%)	0	100	100
1	CCC	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
2	BBB	155/155 (100%)	143 (92%)	12 (8%)	0	100	100
2	DDD	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
All	All	618/622 (99%)	585 (95%)	33 (5%)	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	AAA	143/141 (101%)	138 (96%)	5 (4%)	31	51
1	CCC	141/141 (100%)	135 (96%)	6 (4%)	25	42
2	BBB	142/140 (101%)	133 (94%)	9 (6%)	15	25
2	DDD	140/140 (100%)	135 (96%)	5 (4%)	30	49
All	All	566/562 (101%)	541 (96%)	25 (4%)	25	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	-7	LEU
1	AAA	29	SER
1	AAA	60	LYS
1	AAA	144	MET
1	AAA	147	SER
2	BBB	-7	LEU
2	BBB	-6	ILE
2	BBB	39	GLN
2	BBB	114	THR
2	BBB	129	GLU
2	BBB	130[A]	ASN
2	BBB	130[B]	ASN
2	BBB	145	GLN
2	BBB	146	VAL
1	CCC	-7	LEU
1	CCC	-6	ILE
1	CCC	58	PHE
1	CCC	75	GLU
1	CCC	118	LYS
1	CCC	127	GLN
2	DDD	5	ASN
2	DDD	9	THR
2	DDD	14	GLN
2	DDD	21	ILE
2	DDD	43	THR

Sometimes 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	CCC	601	-	2,2,2	0.39	0	1,1,1	0.06	0
3	FMT	DDD	602	-	2,2,2	0.31	0	1,1,1	0.18	0
4	PEG	AAA	804	-	6,6,6	0.32	0	5,5,5	0.46	0
3	FMT	BBB	403	-	2,2,2	0.34	0	1,1,1	0.12	0
3	FMT	AAA	803	-	2,2,2	0.30	0	1,1,1	0.18	0
3	FMT	BBB	401	-	2,2,2	0.29	0	1,1,1	0.15	0
3	FMT	CCC	602	-	2,2,2	0.32	0	1,1,1	0.14	0
3	FMT	DDD	601	-	2,2,2	0.28	0	1,1,1	0.14	0
3	FMT	AAA	801	-	2,2,2	0.42	0	1,1,1	0.06	0
3	FMT	BBB	402	-	2,2,2	0.31	0	1,1,1	0.13	0
3	FMT	AAA	805	-	2,2,2	0.29	0	1,1,1	0.14	0
3	FMT	AAA	802	-	2,2,2	0.27	0	1,1,1	0.18	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
4	PEG	AAA	804	-	-	4/4/4/4	-

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
4	AAA	804	PEG	C1-C2-O2-C3
4	AAA	804	PEG	C4-C3-O2-C2
4	AAA	804	PEG	O2-C3-C4-O4
4	AAA	804	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	601	FMT	1	0
3	DDD	602	FMT	1	0
4	AAA	804	PEG	30	0
3	AAA	803	FMT	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	AAA	156/156 (100%)	-0.01	1 (0%)	85	83	21, 54, 80, 91	2 (1%)
1	CCC	156/156 (100%)	-0.11	2 (1%)	74	71	37, 55, 80, 106	0
2	BBB	155/155 (100%)	0.10	0	100	100	28, 61, 83, 97	2 (1%)
2	DDD	155/155 (100%)	0.26	2 (1%)	74	71	49, 71, 92, 103	0
All	All	622/622 (100%)	0.06	5 (0%)	82	80	21, 59, 87, 106	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	89	GLY	2.6
2	DDD	17	PHE	2.6
1	CCC	148	ILE	2.4
1	CCC	-7	LEU	2.2
2	DDD	115	PHE	2.1

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 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
3	FMT	BBB	402	3/3	0.57	0.13	88,88,89,92	0
3	FMT	DDD	602	3/3	0.71	0.13	109,109,109,111	0
3	FMT	AAA	803	3/3	0.75	0.15	84,84,85,88	0
3	FMT	CCC	602	3/3	0.76	0.12	73,73,74,75	0
3	FMT	BBB	401	3/3	0.78	0.11	84,84,89,89	0
3	FMT	DDD	601	3/3	0.83	0.09	77,77,79,83	0
4	PEG	AAA	804	7/7	0.86	0.18	41,42,42,43	7
3	FMT	AAA	802	3/3	0.88	0.09	72,72,76,77	0
3	FMT	BBB	403	3/3	0.90	0.46	90,90,94,98	0
3	FMT	CCC	601	3/3	0.90	0.22	74,74,75,78	0
3	FMT	AAA	805	3/3	0.91	0.11	76,76,77,78	0
3	FMT	AAA	801	3/3	0.95	0.11	47,47,51,54	0
5	HG	BBB	404	1/1	0.98	0.09	82,82,82,82	1
6	CA	AAA	807	1/1	0.98	0.04	74,74,74,74	1
5	HG	CCC	603	1/1	0.99	0.03	61,61,61,61	1
5	HG	DDD	603	1/1	0.99	0.07	65,65,65,65	1
5	HG	AAA	806	1/1	0.99	0.03	47,47,47,47	1

6.5 Other polymers ⓘ

There are no such residues in this entry.