wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 09:00 PM EDT

PDB ID	:	5MQZ
Title	:	Archaeal branched-chain amino acid aminotransferase from Archaeoglobus fulgidus; holoform
Authors	:	James, P.; Isupov, M.N.; Sayer, C.; Littlechild, J.A.; Sutter, J.M.; Schmidt, M.; Schoenheit, P.
Deposited on	:	2016-12-21
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

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	Percentile Ranks	Value
Rfree		0.218
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		5.1%
RSRZ outliers		3.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
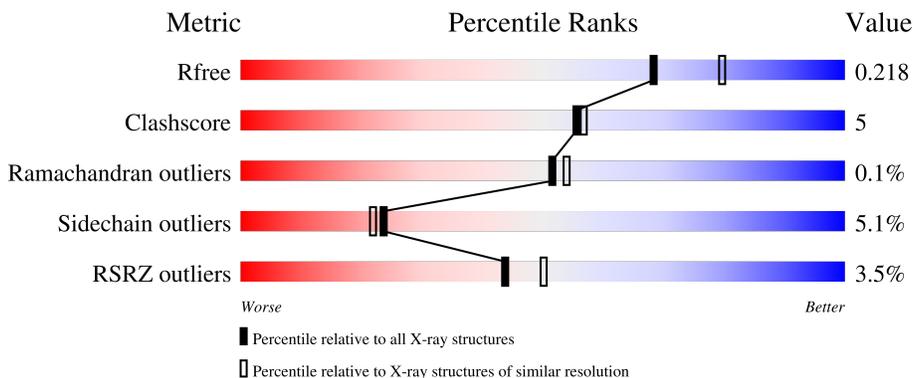
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	290	4% 83% 13% ••
1	B	290	4% 86% 10% ••
1	C	290	2% 86% 11% ••
1	D	290	2% 87% 12% ••
1	E	290	4% 84% 13% ••

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Mol	Chain	Length	Quality of chain
1	F	290	4% ▬ 85% 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	TAM	B	303	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 15167 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 Putative branched-chain-amino-acid aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	30	0
			2460	1580	416	458	1	5			
1	B	286	Total	C	N	O	P	S	0	23	0
			2412	1550	409	447	1	5			
1	C	286	Total	C	N	O	P	S	0	19	0
			2395	1532	410	447	1	5			
1	D	290	Total	C	N	O	P	S	0	15	0
			2396	1534	402	454	1	5			
1	E	287	Total	C	N	O	P	S	0	22	0
			2414	1544	407	457	1	5			
1	F	287	Total	C	N	O	P	S	0	15	0
			2371	1516	399	450	1	5			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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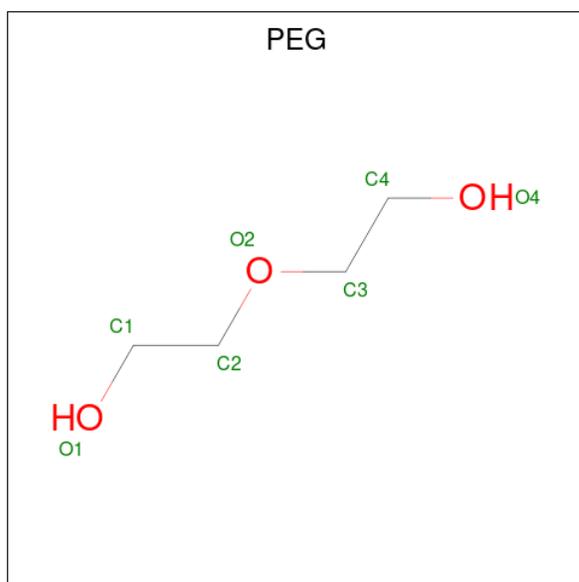
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 4	O 3	0	0
3	D	1	Total 7	C 4	O 3	0	0

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).

TAM
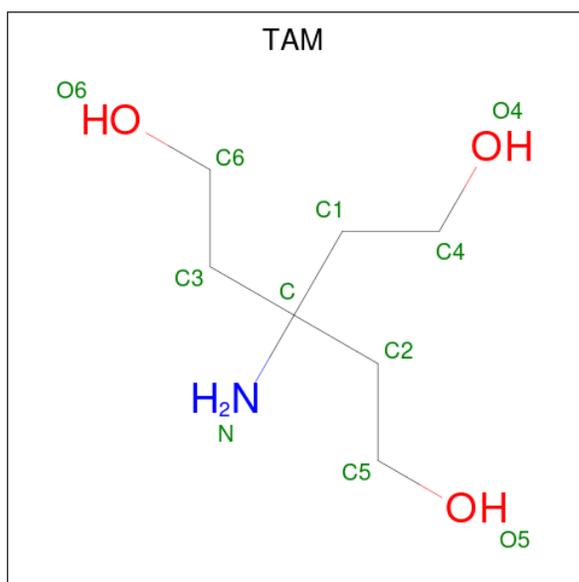
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 11	C 7	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 11	C 7	N 1	O 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
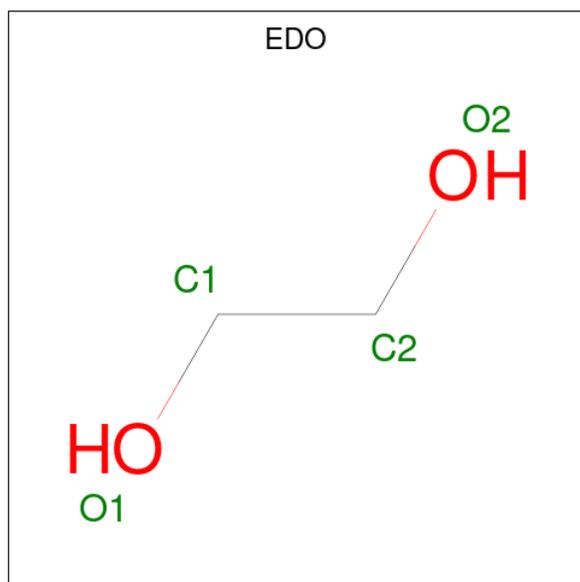
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	116	Total 116	O 116	0	0
6	B	118	Total 118	O 118	0	0
6	C	101	Total 101	O 101	0	0
6	D	122	Total 122	O 122	0	0
6	E	110	Total 110	O 110	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	101	Total 101	O 101	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: Putative branched-chain-amino-acid aminotransferase
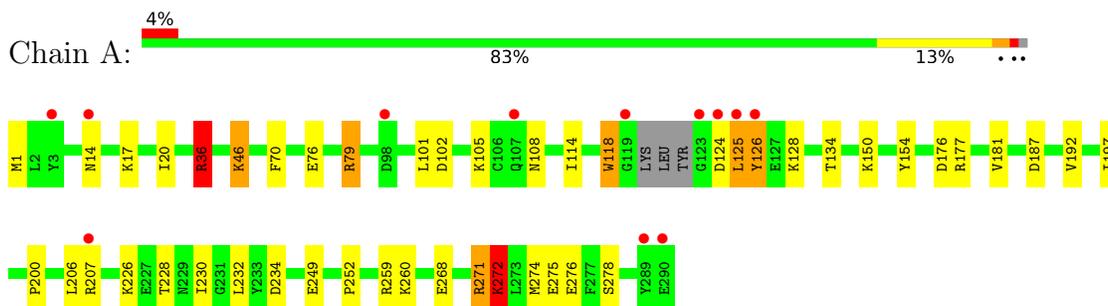
Chain A:

- Molecule 1: Putative branched-chain-amino-acid aminotransferase

Chain B:

- Molecule 1: Putative branched-chain-amino-acid aminotransferase

Chain C:

- Molecule 1: Putative branched-chain-amino-acid aminotransferase

Chain D:

T228 N229 I230 D234 E249 P252 K260 R271 K272 L273 M274 S278 K279 L280 E290

● Molecule 1: Putative branched-chain-amino-acid aminotransferase

Chain E:

4%

84%   13%   ••

M1 K17 R36 F70 E76 R79 R84 D98 K105 C106 Q107 N108 I114 W118 G119 LYS LEU TYR G123 D124 L125 Y126 T134 V137 K150 A172 R177 V181 G184 D187 V192 I197 T198 T202 R207 E212

E216 R220 T228 N229 I230 D234 E249 P252 D257 E268 R271 K272 L273 M274 S278 I288 Y289 E290

● Molecule 1: Putative branched-chain-amino-acid aminotransferase

Chain F:

4%

85%   12%   ••

M1 N14 K17 I20 I35 R36 A37 Y38 N39 R44 L45 K46 I49 F70 R79 R84 I88 I96 G97 D98 K105 C106 Q107 N108 W118 G119 LYS LEU TYR G123 D124 L125 Y126 E127 A144 K150 K161 N165 R177 V181

D187 V192 I197 R207 R220 I230 D234 E249 P252 K260 E268 R271 K272 L273 M274 S278 E290
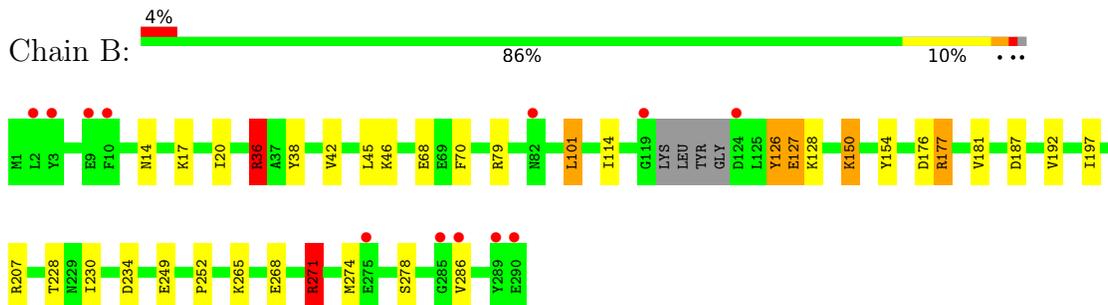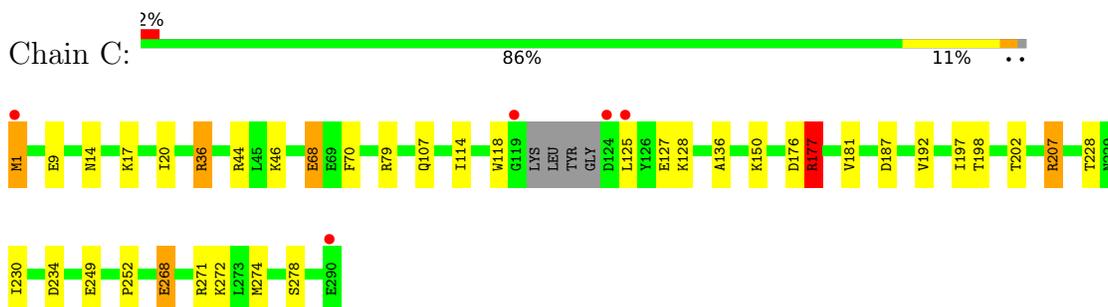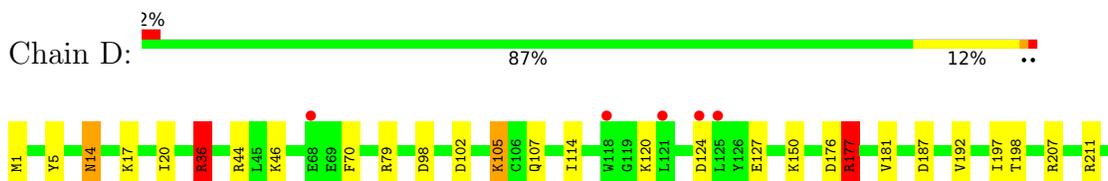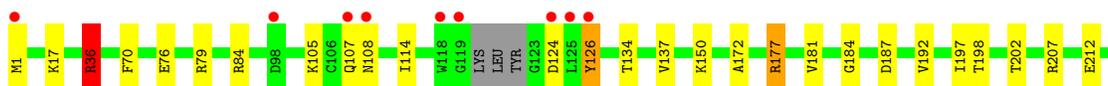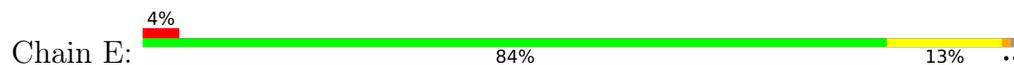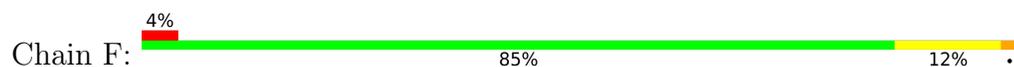
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.92Å 139.12Å 167.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.86 – 2.10 69.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.86-2.10) 99.8 (69.56-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155, BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.181 , 0.218 0.181 , 0.218	Depositor DCC
R_{free} test set	4801 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.9	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	0.97	EDS
Total number of atoms	15167	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: CL, EDO, PEG, TAM, LLP

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	0.71	0/2559	1.03	15/3450 (0.4%)
1	B	0.68	0/2496	0.95	16/3367 (0.5%)
1	C	0.70	0/2458	0.93	11/3317 (0.3%)
1	D	0.75	2/2452 (0.1%)	0.95	12/3315 (0.4%)
1	E	0.72	0/2486	0.92	7/3357 (0.2%)
1	F	0.69	0/2425	0.91	9/3276 (0.3%)
All	All	0.71	2/14876 (0.0%)	0.95	70/20082 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107[A]	GLN	CD-NE2	7.51	1.51	1.32
1	D	107[B]	GLN	CD-NE2	7.51	1.51	1.32

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271[A]	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	A	271[B]	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	C	36[A]	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	C	36[B]	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	A	79	ARG	NE-CZ-NH2	-10.22	115.19	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68[A]	GLU	Mainchain
1	C	68[B]	GLU	Mainchain

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	2460	0	2569	37	0
1	B	2412	0	2513	30	0
1	C	2395	0	2471	23	0
1	D	2396	0	2449	20	0
1	E	2414	0	2479	30	0
1	F	2371	0	2419	25	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	7	0	10	2	0
3	D	7	0	10	1	0
4	A	11	0	17	2	0
4	B	11	0	17	1	0
5	B	8	0	12	0	0
5	D	4	0	6	0	0
6	A	116	0	0	6	0
6	B	118	0	0	4	0
6	C	101	0	0	2	0
6	D	122	0	0	2	0
6	E	110	0	0	2	0
6	F	101	0	0	3	0
All	All	15167	0	14972	150	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 5.

The worst 5 of 150 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:F:220[B]:ARG:HH11	1:F:220[B]:ARG:HG3	1.39	0.88
1:B:268[B]:GLU:HG3	1:B:271[B]:ARG:NH1	1.90	0.85
1:A:181:VAL:HB	1:A:230[A]:ILE:HG13	1.57	0.83
1:A:101[B]:LEU:HD21	1:B:154:TYR:HD2	1.52	0.72
1:B:150:LLP:H4'1	6:B:431:HOH:O	1.89	0.71

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	312/290 (108%)	304 (97%)	8 (3%)	0	100	100
1	B	304/290 (105%)	296 (97%)	8 (3%)	0	100	100
1	C	300/290 (103%)	292 (97%)	8 (3%)	0	100	100
1	D	302/290 (104%)	293 (97%)	9 (3%)	0	100	100
1	E	304/290 (105%)	296 (97%)	8 (3%)	0	100	100
1	F	297/290 (102%)	288 (97%)	7 (2%)	2 (1%)	22	18
All	All	1819/1740 (104%)	1769 (97%)	48 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	108[A]	ASN
1	F	108[B]	ASN

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	271/244 (111%)	254 (94%)	17 (6%)	18	15
1	B	264/244 (108%)	250 (95%)	14 (5%)	22	20
1	C	260/244 (107%)	243 (94%)	17 (6%)	17	14
1	D	259/244 (106%)	244 (94%)	15 (6%)	20	17
1	E	263/244 (108%)	250 (95%)	13 (5%)	25	23
1	F	256/244 (105%)	239 (93%)	17 (7%)	16	14
All	All	1573/1464 (107%)	1480 (94%)	93 (6%)	24	17

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	177[A]	ARG
1	E	177[B]	ARG
1	D	187	ASP
1	E	36[B]	ARG
1	E	290	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	229	ASN
1	F	14	ASN
1	F	165	ASN
1	F	157	ASN
1	D	205	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	D	150	1	23,24,25	2.90	5 (21%)	25,32,34	1.98	9 (36%)
1	LLP	A	150	1	23,24,25	2.92	5 (21%)	25,32,34	1.99	9 (36%)
1	LLP	B	150	1	23,24,25	2.93	5 (21%)	25,32,34	1.93	9 (36%)
1	LLP	E	150	1	23,24,25	2.96	5 (21%)	25,32,34	1.96	8 (32%)
1	LLP	F	150	1	23,24,25	2.93	5 (21%)	25,32,34	1.92	9 (36%)
1	LLP	C	150	1	23,24,25	2.95	5 (21%)	25,32,34	1.99	8 (32%)

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	D	150	1	-	4/16/17/19	0/1/1/1
1	LLP	A	150	1	-	4/16/17/19	0/1/1/1
1	LLP	B	150	1	-	4/16/17/19	0/1/1/1
1	LLP	E	150	1	-	4/16/17/19	0/1/1/1
1	LLP	F	150	1	-	5/16/17/19	0/1/1/1
1	LLP	C	150	1	-	5/16/17/19	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	LLP	C3-C2	8.46	1.49	1.40
1	F	150	LLP	C3-C2	8.31	1.49	1.40
1	E	150	LLP	C3-C2	8.30	1.49	1.40
1	B	150	LLP	C3-C2	8.28	1.49	1.40
1	A	150	LLP	C3-C2	7.99	1.48	1.40

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	LLP	C4-C4'-NZ	-4.03	105.80	124.31
1	E	150	LLP	C4-C4'-NZ	-3.94	106.21	124.31
1	F	150	LLP	C4-C4'-NZ	-3.93	106.26	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	150	LLP	C4-C4'-NZ	-3.91	106.35	124.31
1	B	150	LLP	C4-C4'-NZ	-3.85	106.61	124.31

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	150	LLP	C4-C4'-NZ-CE
1	B	150	LLP	C4-C4'-NZ-CE
1	C	150	LLP	C4-C4'-NZ-CE
1	C	150	LLP	O-C-CA-CB
1	D	150	LLP	C4-C4'-NZ-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	150	LLP	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	#$|Z| > 2$
5	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.56	0
4	TAM	B	303	-	7,10,10	0.31	0	9,12,12	1.15	0
3	PEG	D	301	-	6,6,6	0.37	0	5,5,5	0.59	0
5	EDO	B	302	-	3,3,3	0.47	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
4	TAM	A	303	-	7,10,10	0.47	0	9,12,12	0.67	0
3	PEG	A	302	-	6,6,6	0.48	0	5,5,5	0.37	0
5	EDO	B	301	-	3,3,3	0.42	0	2,2,2	0.69	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
5	EDO	D	302	-	-	0/1/1/1	-
4	TAM	B	303	-	-	4/12/12/12	-
3	PEG	D	301	-	-	2/4/4/4	-
5	EDO	B	302	-	-	0/1/1/1	-
4	TAM	A	303	-	-	6/12/12/12	-
3	PEG	A	302	-	-	3/4/4/4	-
5	EDO	B	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	TAM	C2-C-C1-C4
4	A	303	TAM	N-C-C1-C4
4	A	303	TAM	C1-C-C3-C6
4	A	303	TAM	N-C-C3-C6
4	B	303	TAM	C1-C-C3-C6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	TAM	1	0
3	D	301	PEG	1	0
4	A	303	TAM	2	0
3	A	302	PEG	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, 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	286/290 (98%)	0.22	12 (4%)	36	42	25, 41, 71, 140	0
1	B	285/290 (98%)	0.27	12 (4%)	36	42	25, 40, 70, 128	0
1	C	285/290 (98%)	0.20	5 (1%)	68	72	25, 41, 76, 118	0
1	D	289/290 (99%)	0.16	7 (2%)	59	64	25, 38, 78, 121	0
1	E	286/290 (98%)	0.32	12 (4%)	36	42	25, 39, 77, 150	0
1	F	286/290 (98%)	0.32	12 (4%)	36	42	27, 41, 75, 137	0
All	All	1717/1740 (98%)	0.25	60 (3%)	44	50	25, 40, 77, 150	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	124	ASP	8.7
1	F	123	GLY	6.1
1	B	124	ASP	5.5
1	F	119	GLY	5.2
1	F	124	ASP	4.9

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	LLP	C	150	24/25	0.95	0.14	30,40,56,67	0
1	LLP	B	150	24/25	0.96	0.13	28,37,54,69	0
1	LLP	D	150	24/25	0.96	0.14	29,38,52,65	0
1	LLP	E	150	24/25	0.96	0.12	31,38,54,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	LLP	A	150	24/25	0.97	0.13	31,40,52,73	0
1	LLP	F	150	24/25	0.97	0.12	30,39,52,62	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å²)	Q<0.9
5	EDO	B	301	4/4	0.71	0.35	62,70,71,76	4
4	TAM	B	303	11/11	0.73	0.46	51,59,73,83	11
4	TAM	A	303	11/11	0.79	0.37	52,63,76,76	11
5	EDO	D	302	4/4	0.85	0.25	41,44,49,56	4
5	EDO	B	302	4/4	0.86	0.19	62,68,74,78	4
3	PEG	D	301	7/7	0.86	0.38	60,67,73,81	7
3	PEG	A	302	7/7	0.90	0.20	54,62,72,78	7
2	CL	E	301	1/1	0.99	0.13	33,33,33,33	1
2	CL	A	301	1/1	1.00	0.14	31,31,31,31	1
2	CL	C	301	1/1	1.00	0.11	32,32,32,32	1

6.5 Other polymers ⓘ

There are no such residues in this entry.