wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 11:02 AM EDT

PDB ID	:	1T5E
Title	:	The structure of MexA
Authors	:	Higgins, M.K.; Bokma, E.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on	:	2004-05-04
Resolution	:	3.00 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:

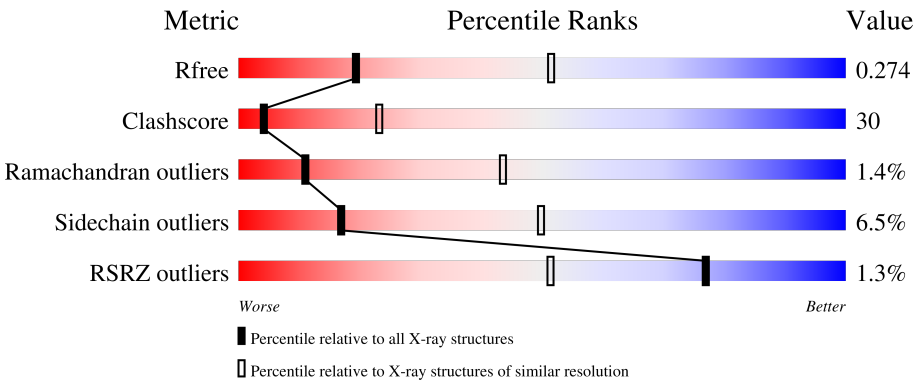
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	360	6%; 36%, 25%, •, 36%
1	B	360	36%, 26%, •, 36%
1	C	360	%; 36%, 26%, •, 36%
1	D	360	35%, 26%, •, 36%
1	E	360	36%, 25%, •, 36%

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Mol	Chain	Length	Quality of chain
1	F	360	% 33% 28% • 36%
1	G	360	2% 34% 27% • 36%
1	H	360	% 34% 27% • 36%
1	I	360	34% 28% • 36%
1	J	360	33% 28% • 36%
1	K	360	33% 28% • • 36%
1	L	360	32% 29% • 36%
1	M	360	% 36% 26% • 36%

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
2	GOL	A	361	-	-	X	-
2	GOL	J	361	-	-	X	-
3	3GR	F	361	-	-	X	-
3	3GR	I	361	-	-	X	-

2 Entry composition (i)

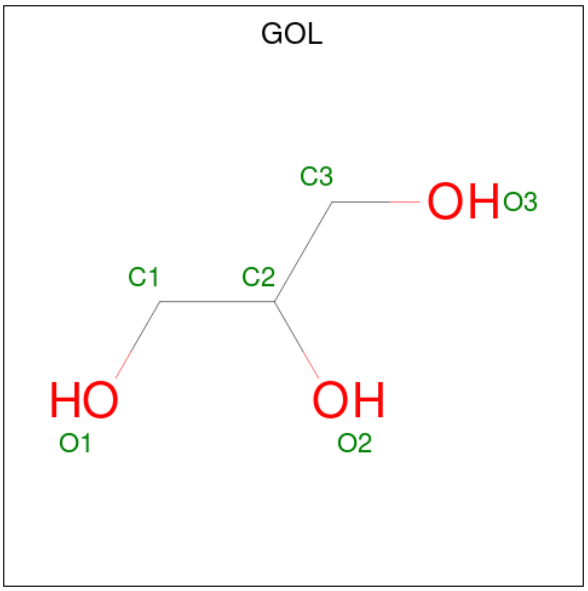
There are 3 unique types of molecules in this entry. The entry contains 23101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance protein mexA.

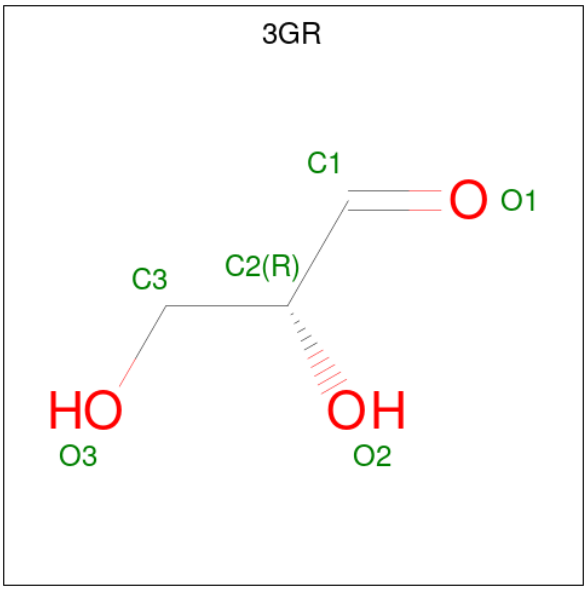
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1771	1101	319	349	2	0	0	0
1	B	231	1771	1101	319	349	2	0	0	0
1	C	231	1771	1101	319	349	2	0	0	0
1	D	231	1771	1101	319	349	2	0	0	0
1	E	231	1771	1101	319	349	2	0	0	0
1	F	231	1771	1101	319	349	2	0	0	0
1	G	231	1771	1101	319	349	2	0	0	0
1	H	231	1771	1101	319	349	2	0	0	0
1	I	231	1771	1101	319	349	2	0	0	0
1	J	231	1771	1101	319	349	2	0	0	0
1	K	231	1771	1101	319	349	2	0	0	0
1	L	231	1771	1101	319	349	2	0	0	0
1	M	231	1771	1101	319	349	2	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	J	1	6	3	3	0	0
2	M	1	6	3	3	0	0

- Molecule 3 is D-Glyceraldehyde (three-letter code: 3GR) (formula: $C_3H_6O_3$).



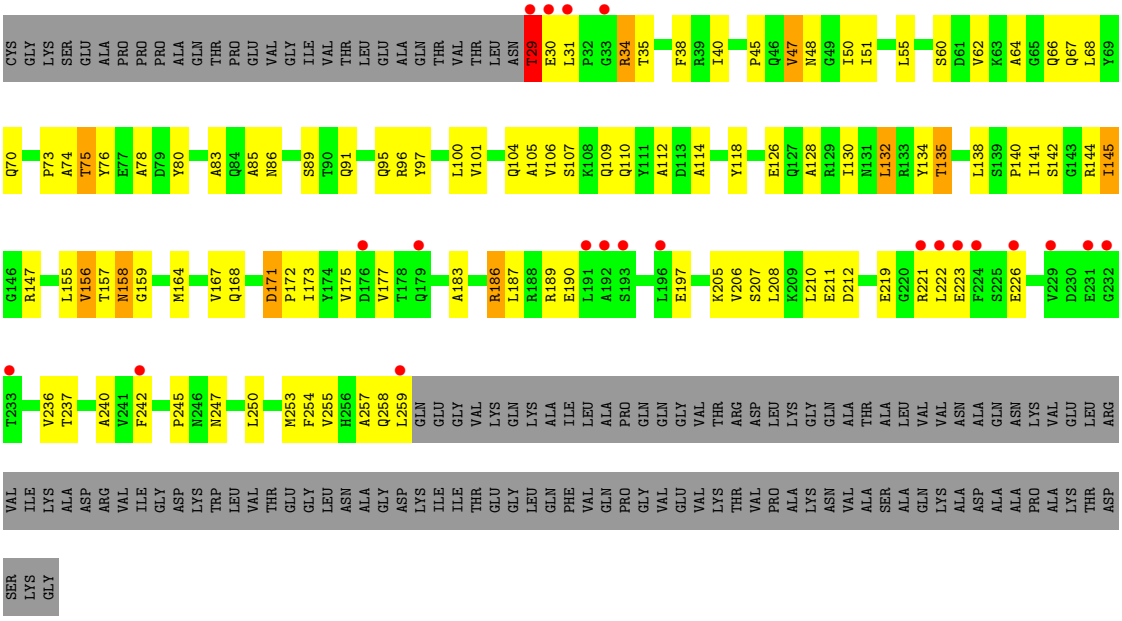
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	6	3	3	0	0
3	D	1	6	3	3	0	0
3	E	1	6	3	3	0	0
3	F	1	6	3	3	0	0
3	G	1	6	3	3	0	0
3	H	1	6	3	3	0	0
3	I	1	6	3	3	0	0
3	K	1	6	3	3	0	0
3	L	1	6	3	3	0	0

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.

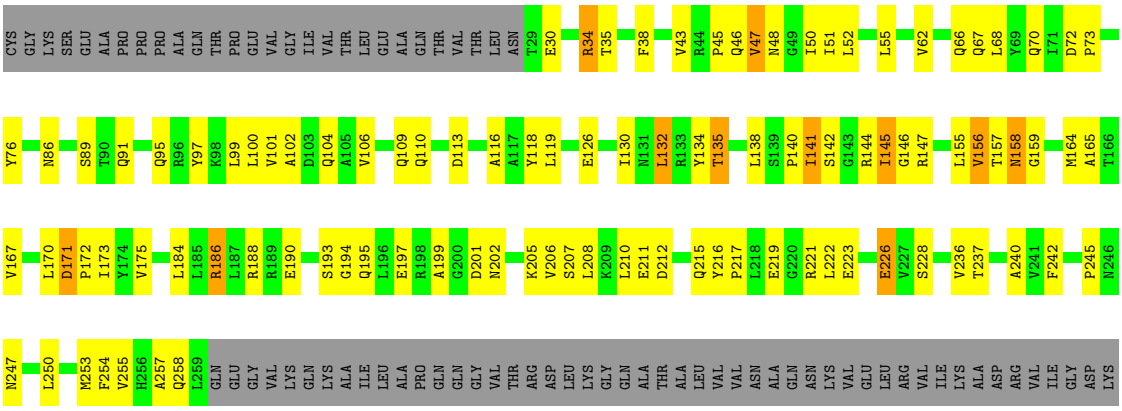
• Molecule 1: Multidrug resistance protein mexA

Chain A: 6% 36% 25% • 36%



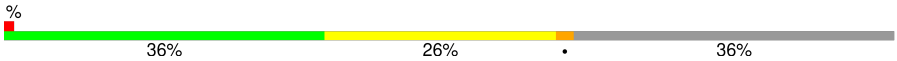
• Molecule 1: Multidrug resistance protein mexA

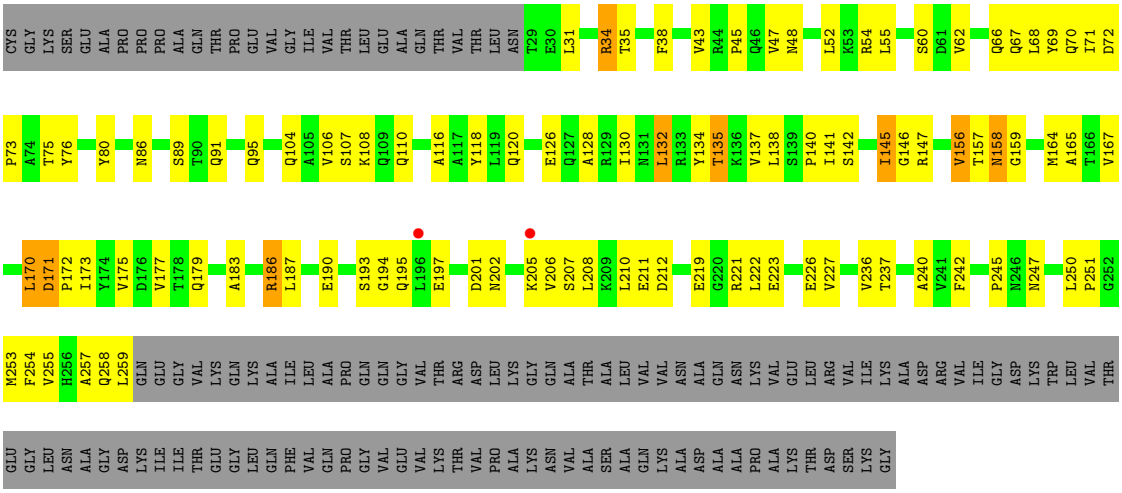
Chain B: 36% 26% • 36%



- Molecule 1: Multidrug resistance protein mexA

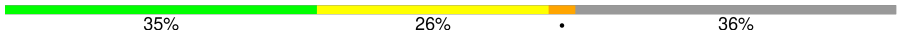
Chain C:

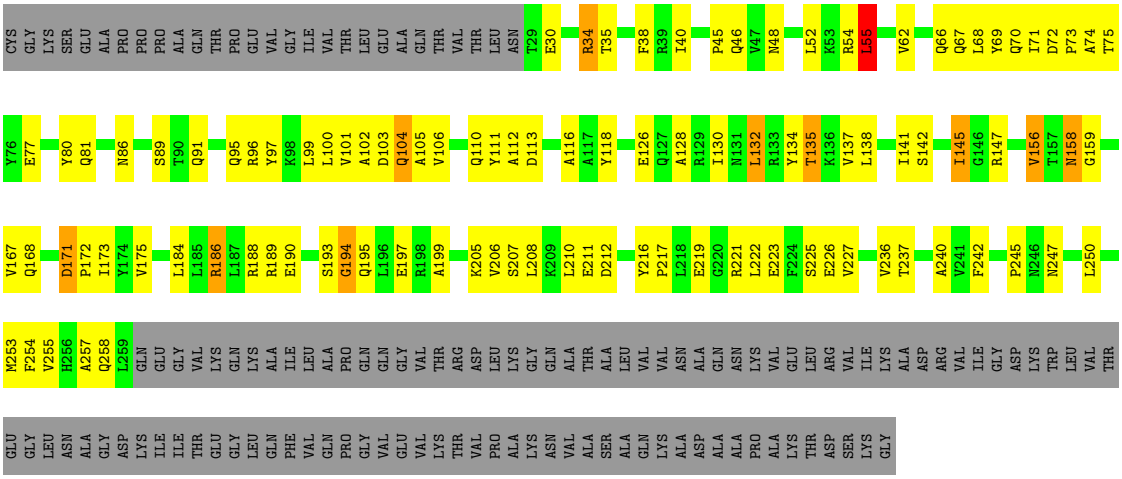




- Molecule 1: Multidrug resistance protein mexA

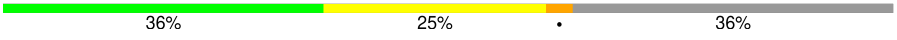
Chain D:

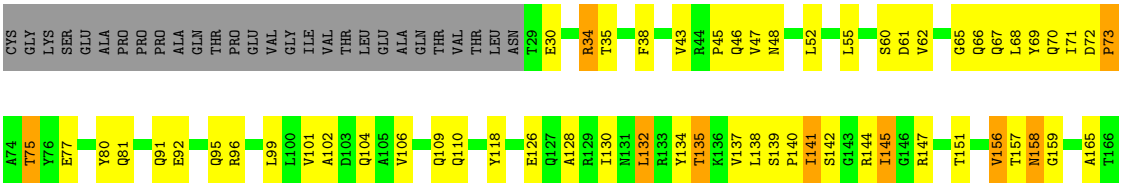


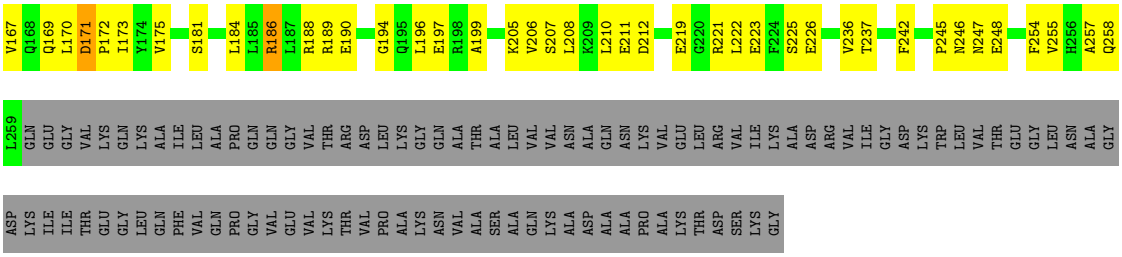


- Molecule 1: Multidrug resistance protein mexA

Chain E:

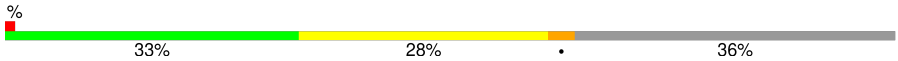


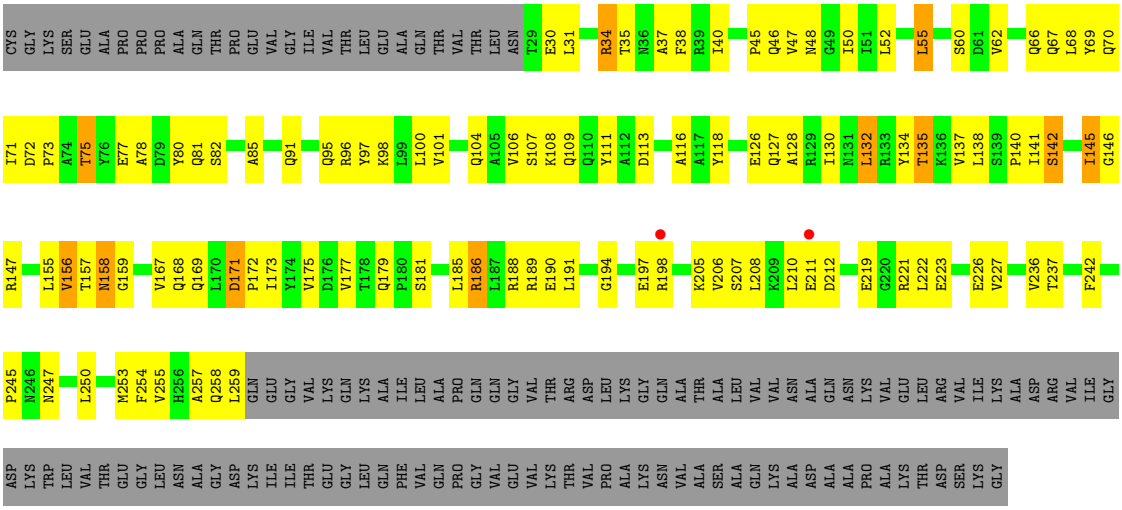




• Molecule 1: Multidrug resistance protein mexA

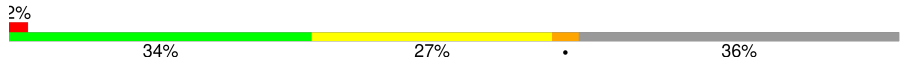
Chain F:

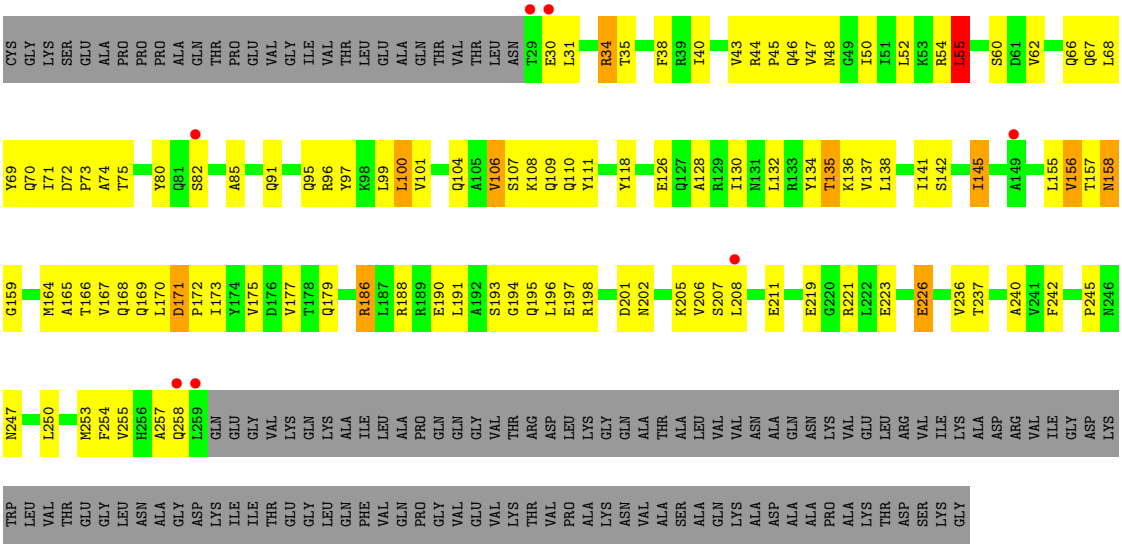




• Molecule 1: Multidrug resistance protein mexA

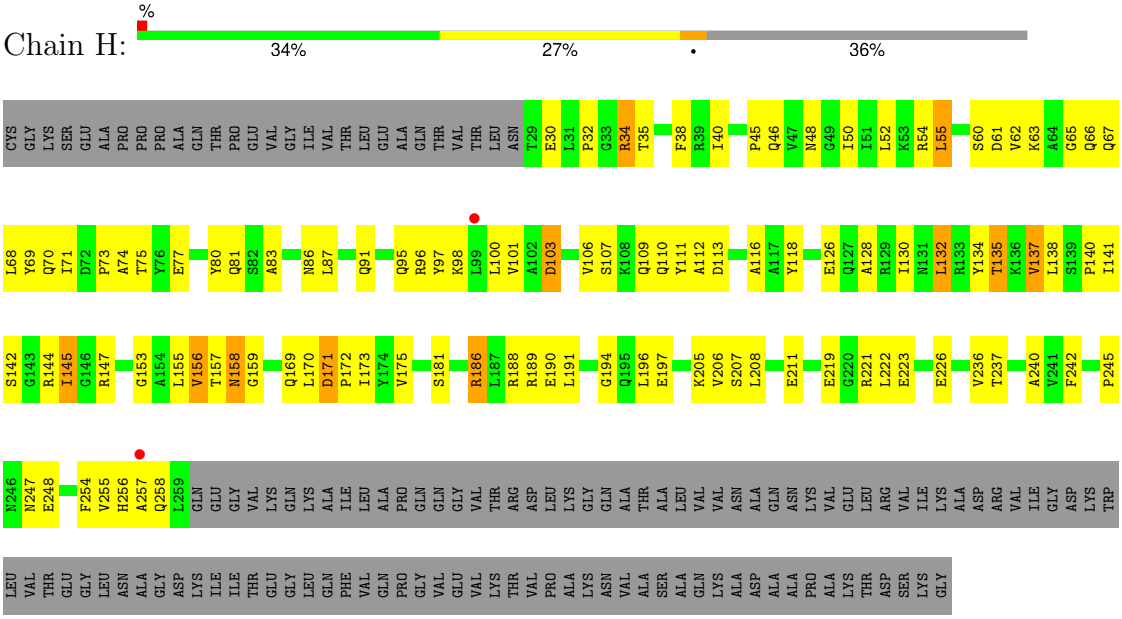
Chain G:





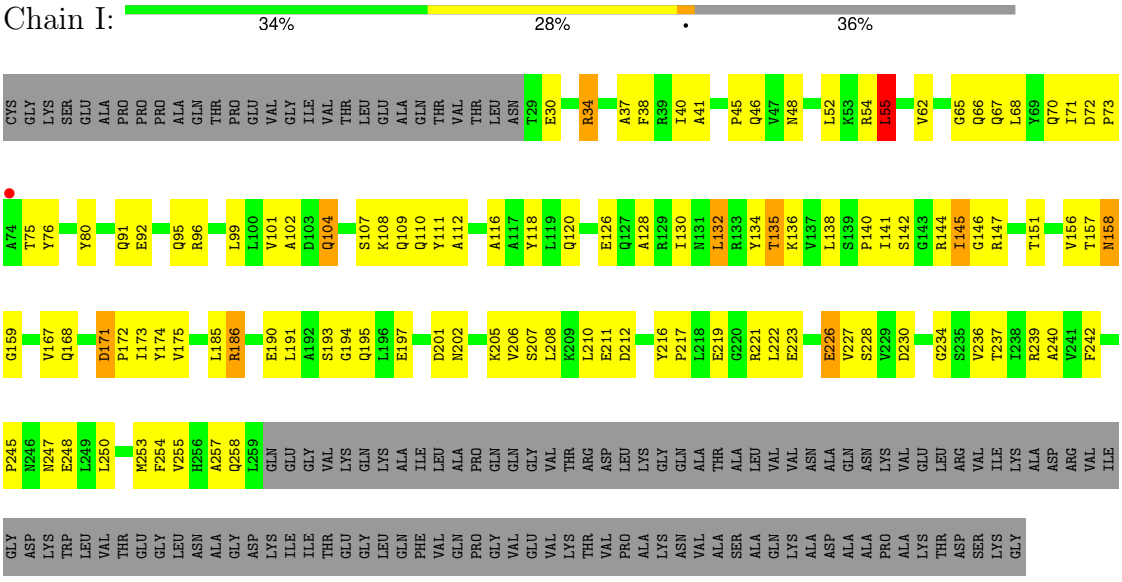
• Molecule 1: Multidrug resistance protein mexA

Chain H:



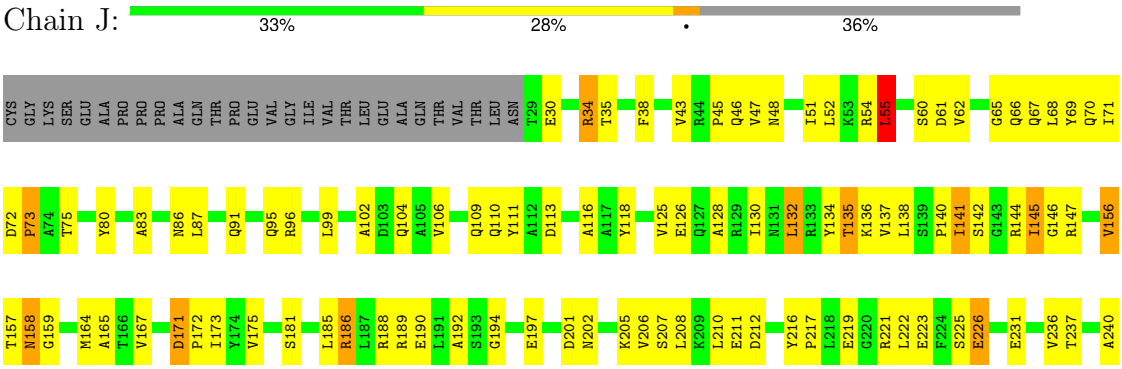
• Molecule 1: Multidrug resistance protein mexA

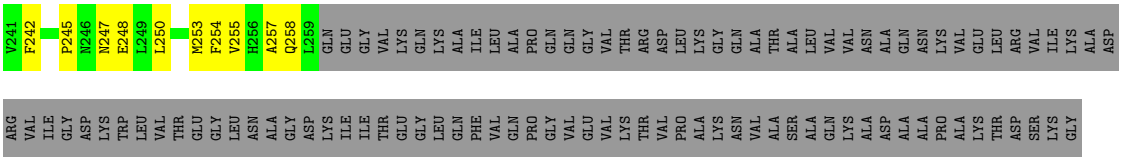
Chain I:



• Molecule 1: Multidrug resistance protein mexA

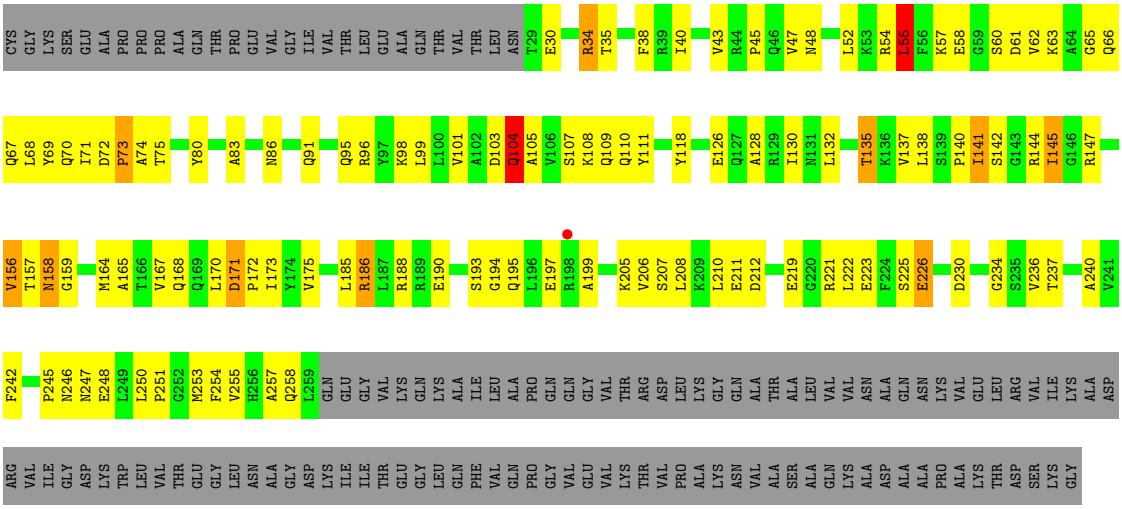
Chain J:





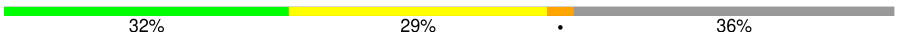
- Molecule 1: Multidrug resistance protein mexA

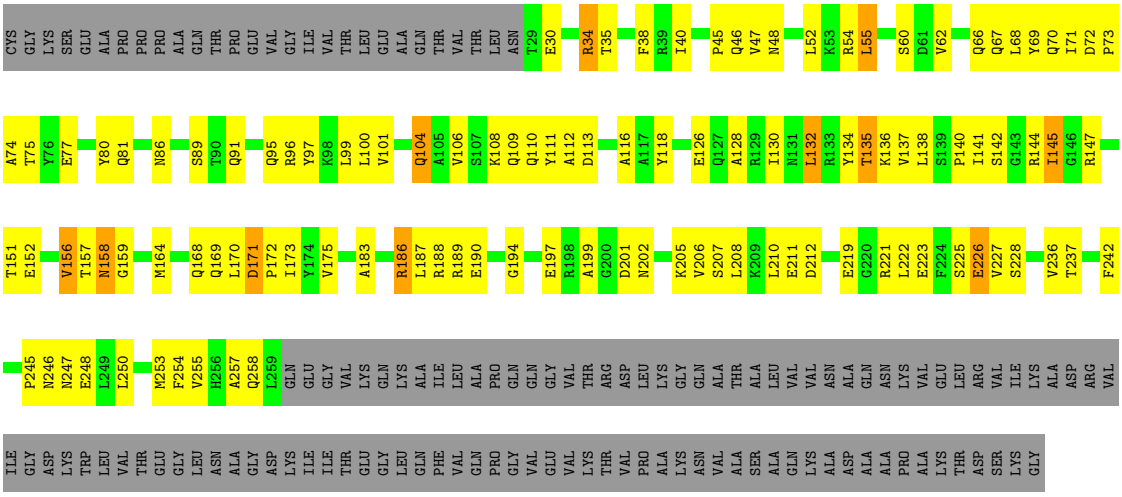
Chain K:



- Molecule 1: Multidrug resistance protein mexA

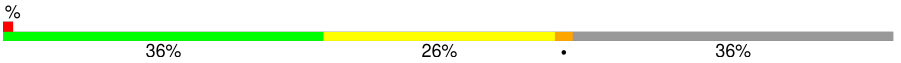
Chain L:

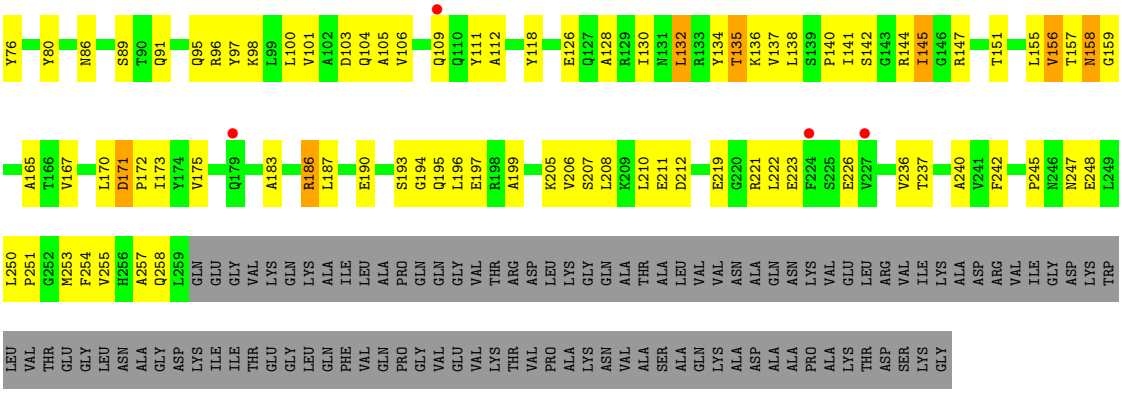




- Molecule 1: Multidrug resistance protein mexA

Chain M:




Y76 Y80 N86 S89 T90 Q91 Q95 R96 Y97 K98 L99 L100 V101 A102 D103 Q104 A105 V106 Q109 Q110 Y111 A112 Y118 E126 Q127 A128 R129 I130 N131 L132 R133 Y134 T135 K136 V137 L138 S139 P140 I141 S142 G143 R144 I145 G146 R147 T151 L155 V156 T157 N158 G159
A165 T166 V167 L170 D171 P172 I173 Y174 V175 Q179 A183 R186 L187 E190 S193 G194 Q195 L196 E197 R198 A199 K205 V206 S207 L208 K209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 V236 T237 A240 V241 F242 P245 N246 N247 E248 L249
L250 P251 G252 M253 F254 V255 H256 A257 Q258 L259 GLN GLU GLY VAL LYS GLN LYS ALA ILE LEU ALA PRO GLN GLN GLY VAL THR ARG ASP LEU LYS GLY GLN ALA THR ALA LEU VAL VAL ASN ALA GLN ASN LYS VAL GLU LEU ARG VAL ILE LYS ALA ASP ARG VAL ILE GLY ASP LYS TRP
LEU VAL THR GLU GLY LEU ASN ALA GLY ASP LYS ILE ILE THR GLU GLY LEU GLN PHE VAL LEU GLN PRO GLY VAL GLU VAL LYS THR VAL PRO ALA LYS ASN VAL ALA SER ALA GLN LYS ALA ASP ALA ALA PRO ALA LYS THR ASP SER LYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.55Å 183.59Å 213.31Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	95.00 – 3.00 83.48 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (95.00-3.00) 98.3 (83.48-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.262 , 0.274	Depositor DCC
R_{free} test set	9310 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23101	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3GR, GOL

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	0.48	1/1795 (0.1%)	0.62	0/2434
1	B	0.39	0/1795	0.65	0/2434
1	C	0.40	0/1795	0.66	0/2434
1	D	0.42	0/1795	0.69	0/2434
1	E	0.47	0/1795	0.71	0/2434
1	F	0.38	0/1795	0.67	0/2434
1	G	0.37	0/1795	0.63	0/2434
1	H	0.45	0/1795	0.70	0/2434
1	I	0.49	0/1795	0.71	0/2434
1	J	0.56	0/1795	0.75	0/2434
1	K	0.52	0/1795	0.73	0/2434
1	L	0.48	0/1795	0.71	0/2434
1	M	0.39	0/1795	0.66	0/2434
All	All	0.45	1/23335 (0.0%)	0.68	0/31642

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	A	0	1
1	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	C-N	-14.50	1.00	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	THR	Mainchain
1	I	111	TYR	Sidechain

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	1771	0	1774	109	1
1	B	1771	0	1775	105	0
1	C	1771	0	1775	98	0
1	D	1771	0	1775	110	1
1	E	1771	0	1775	102	0
1	F	1771	0	1775	109	0
1	G	1771	0	1775	120	0
1	H	1771	0	1775	109	0
1	I	1771	0	1775	115	0
1	J	1771	0	1775	110	0
1	K	1771	0	1775	120	0
1	L	1771	0	1775	127	0
1	M	1771	0	1775	110	0
2	A	6	0	8	5	0
2	B	6	0	5	3	0
2	J	6	0	5	5	0
2	M	6	0	5	2	0
3	C	6	0	5	2	0
3	D	6	0	5	0	0
3	E	6	0	5	2	0
3	F	6	0	5	4	0
3	G	6	0	5	1	0
3	H	6	0	5	2	0
3	I	6	0	5	4	0
3	K	6	0	5	3	0
3	L	6	0	5	1	0
All	All	23101	0	23142	1365	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 1365 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:146:GLY:HA3	3:F:361:3GR:O2	1.37	1.24
1:M:70:GLN:HE22	1:M:135:THR:HG23	1.08	1.15
1:A:70:GLN:HE22	1:A:135:THR:HG23	1.18	1.07
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.21	1.05
1:J:91:GLN:HG2	1:J:95:GLN:HE21	1.16	1.04

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:NH2	1:D:194:GLY:O[2_656]	2.19	0.01

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	229/360 (64%)	207 (90%)	21 (9%)	1 (0%)	34 72
1	B	229/360 (64%)	203 (89%)	24 (10%)	2 (1%)	17 55
1	C	229/360 (64%)	209 (91%)	18 (8%)	2 (1%)	17 55
1	D	229/360 (64%)	200 (87%)	24 (10%)	5 (2%)	6 31
1	E	229/360 (64%)	211 (92%)	15 (7%)	3 (1%)	12 45
1	F	229/360 (64%)	209 (91%)	17 (7%)	3 (1%)	12 45
1	G	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	9 39
1	H	229/360 (64%)	205 (90%)	19 (8%)	5 (2%)	6 31
1	I	229/360 (64%)	210 (92%)	16 (7%)	3 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	229/360 (64%)	208 (91%)	17 (7%)	4 (2%)	9	39
1	K	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	9	39
1	L	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	9	39
1	M	229/360 (64%)	204 (89%)	22 (10%)	3 (1%)	12	45
All	All	2977/4680 (64%)	2681 (90%)	253 (8%)	43 (1%)	11	43

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	B	171	ASP
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/287 (65%)	176 (95%)	10 (5%)	22	57
1	B	186/287 (65%)	175 (94%)	11 (6%)	19	54
1	C	186/287 (65%)	176 (95%)	10 (5%)	22	57
1	D	186/287 (65%)	173 (93%)	13 (7%)	15	47
1	E	186/287 (65%)	170 (91%)	16 (9%)	10	37
1	F	186/287 (65%)	173 (93%)	13 (7%)	15	47
1	G	186/287 (65%)	175 (94%)	11 (6%)	19	54
1	H	186/287 (65%)	174 (94%)	12 (6%)	17	50
1	I	186/287 (65%)	176 (95%)	10 (5%)	22	57
1	J	186/287 (65%)	171 (92%)	15 (8%)	11	40
1	K	186/287 (65%)	171 (92%)	15 (8%)	11	40
1	L	186/287 (65%)	174 (94%)	12 (6%)	17	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	186/287 (65%)	177 (95%)	9 (5%)	25	62
All	All	2418/3731 (65%)	2261 (94%)	157 (6%)	17	50

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	145	ILE
1	L	156	VAL
1	J	225	SER
1	K	145	ILE
1	M	135	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	169	GLN
1	J	95	GLN
1	I	36	ASN
1	I	158	ASN
1	K	48	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
3	3GR	H	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.97	1 (25%)
2	GOL	J	361	1	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)
2	GOL	B	361	-	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)
3	3GR	I	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	G	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	E	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.96	1 (25%)
3	3GR	L	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.97	1 (25%)
3	3GR	K	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.97	1 (25%)
3	3GR	D	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.97	1 (25%)
2	GOL	A	361	-	5,5,5	0.23	0	5,5,5	0.49	0
3	3GR	C	361	-	4,5,5	6.16	2 (50%)	4,5,5	14.98	1 (25%)
3	3GR	F	361	-	4,5,5	6.15	2 (50%)	4,5,5	14.96	1 (25%)
2	GOL	M	361	1	5,5,5	4.79	1 (20%)	5,5,5	4.47	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3GR	H	361	-	-	1/3/4/4	-
2	GOL	J	361	1	-	0/4/4/4	-
2	GOL	B	361	-	-	0/4/4/4	-
3	3GR	I	361	-	-	1/3/4/4	-
3	3GR	G	361	-	-	1/3/4/4	-
3	3GR	E	361	-	-	1/3/4/4	-
3	3GR	L	361	-	-	1/3/4/4	-
3	3GR	K	361	-	-	1/3/4/4	-
3	3GR	D	361	-	-	1/3/4/4	-
2	GOL	A	361	-	-	0/4/4/4	-
3	3GR	C	361	-	-	1/3/4/4	-
3	3GR	F	361	-	-	1/3/4/4	-
2	GOL	M	361	1	-	0/4/4/4	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	361	3GR	O3-C3	-10.68	0.97	1.42
3	I	361	3GR	O3-C3	-10.67	0.97	1.42
3	H	361	3GR	O3-C3	-10.67	0.97	1.42
3	L	361	3GR	O3-C3	-10.67	0.97	1.42
2	M	361	GOL	O3-C3	-10.66	0.97	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	361	3GR	O3-C3-C2	29.94	155.34	112.39
3	K	361	3GR	O3-C3-C2	29.93	155.32	112.39
3	D	361	3GR	O3-C3-C2	29.92	155.32	112.39
3	H	361	3GR	O3-C3-C2	29.92	155.32	112.39
3	L	361	3GR	O3-C3-C2	29.92	155.31	112.39

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	361	3GR	O2-C2-C3-O3
3	D	361	3GR	O2-C2-C3-O3
3	E	361	3GR	O2-C2-C3-O3
3	F	361	3GR	O2-C2-C3-O3
3	G	361	3GR	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	361	3GR	2	0
2	J	361	GOL	5	0
2	B	361	GOL	3	0
3	I	361	3GR	4	0
3	G	361	3GR	1	0
3	E	361	3GR	2	0
3	L	361	3GR	1	0
3	K	361	3GR	3	0
2	A	361	GOL	5	0
3	C	361	3GR	2	0
3	F	361	3GR	4	0
2	M	361	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	29:THR	C	30:GLU	N	1.00

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	A	231/360 (64%)	0.47	21 (9%)	9	3	56, 93, 132, 143	2 (0%)
1	B	231/360 (64%)	0.08	0	100	100	37, 80, 110, 123	2 (0%)
1	C	231/360 (64%)	0.06	2 (0%)	84	63	39, 77, 111, 116	2 (0%)
1	D	231/360 (64%)	0.10	0	100	100	30, 82, 109, 123	2 (0%)
1	E	231/360 (64%)	0.01	0	100	100	22, 61, 95, 111	2 (0%)
1	F	231/360 (64%)	0.07	2 (0%)	84	63	53, 80, 106, 111	2 (0%)
1	G	231/360 (64%)	0.15	7 (3%)	50	22	51, 86, 118, 126	2 (0%)
1	H	231/360 (64%)	0.10	2 (0%)	84	63	28, 64, 98, 109	2 (0%)
1	I	231/360 (64%)	0.15	1 (0%)	92	79	24, 62, 96, 109	2 (0%)
1	J	231/360 (64%)	0.06	0	100	100	15, 48, 84, 100	2 (0%)
1	K	231/360 (64%)	0.02	1 (0%)	92	79	20, 59, 92, 107	2 (0%)
1	L	231/360 (64%)	0.03	0	100	100	25, 63, 102, 115	2 (0%)
1	M	231/360 (64%)	0.22	4 (1%)	70	41	40, 93, 117, 130	2 (0%)
All	All	3003/4680 (64%)	0.12	40 (1%)	77	51	15, 75, 114, 143	26 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	4.7
1	M	227	VAL	4.6
1	A	29	THR	3.5
1	A	231	GLU	3.5
1	A	31	LEU	3.2

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
2	GOL	A	361	6/6	0.66	0.33	97,98,99,102	0
3	3GR	F	361	6/6	0.69	0.27	99,100,101,103	0
2	GOL	J	361	6/6	0.71	0.40	92,94,94,96	0
3	3GR	E	361	6/6	0.77	0.37	93,95,98,102	0
2	GOL	B	361	6/6	0.78	0.30	95,96,96,96	0
3	3GR	C	361	6/6	0.79	0.30	100,100,101,102	0
3	3GR	H	361	6/6	0.80	0.32	87,88,89,90	0
3	3GR	G	361	6/6	0.81	0.21	103,104,105,106	0
2	GOL	M	361	6/6	0.82	0.26	99,100,101,101	0
3	3GR	K	361	6/6	0.82	0.36	79,80,83,84	0
3	3GR	I	361	6/6	0.86	0.30	87,87,88,88	0
3	3GR	L	361	6/6	0.86	0.35	81,82,83,86	0
3	3GR	D	361	6/6	0.89	0.32	93,93,94,95	0

6.5 Other polymers (i)

There are no such residues in this entry.