



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 11:36 AM UTC

PDB ID : 1T5E / pdb_00001t5e
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 ⓘ 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

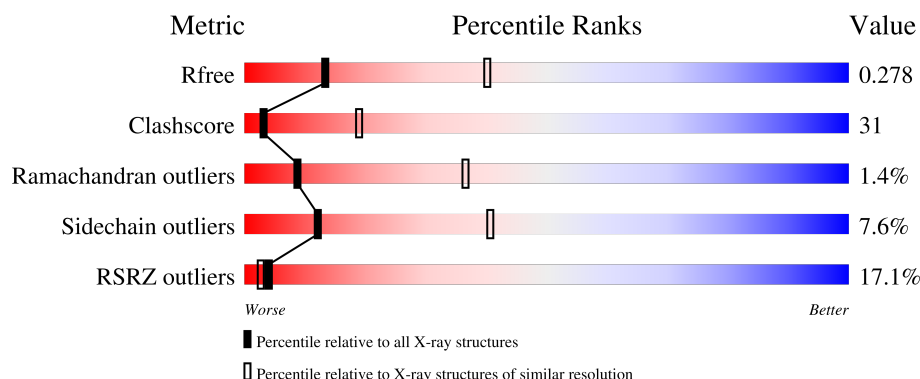
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	360	18% 32% 28% • • 36%
1	B	360	13% 34% 27% • 36%
1	C	360	10% 34% 27% • 36%
1	D	360	12% 32% 27% • • 36%
1	E	360	5% 34% 27% • • 36%

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Mol	Chain	Length	Quality of chain
1	F	360	
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	

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	X
2	GOL	B	361	-	-	-	X
2	GOL	J	361	-	-	X	-
3	3GR	C	361	-	-	-	X
3	3GR	D	361	-	-	-	X
3	3GR	E	361	-	-	-	X
3	3GR	F	361	-	-	X	X
3	3GR	G	361	-	-	-	X
3	3GR	H	361	-	-	-	X
3	3GR	I	361	-	-	X	-
3	3GR	K	361	-	-	-	X

2 Entry composition

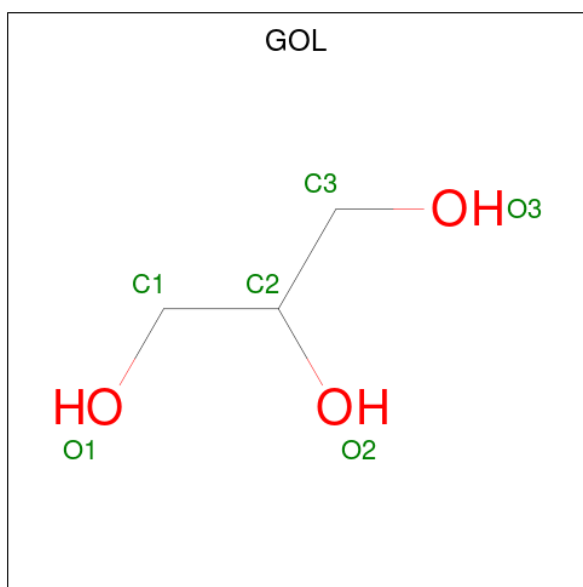
There are 3 unique types of molecules in this entry. The entry contains 23101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

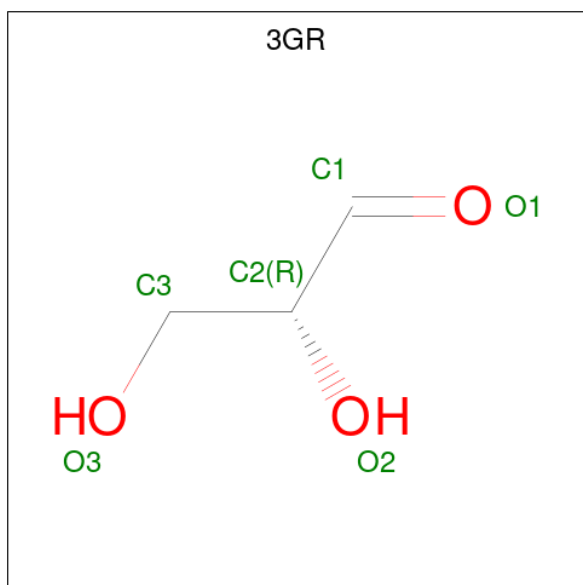
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	B	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	C	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	D	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	E	231	Total	C	N	O	S	0	0	0
			1771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

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is D-Glyceraldehyde (CCD ID: 3GR) (formula: $C_3H_6O_3$).

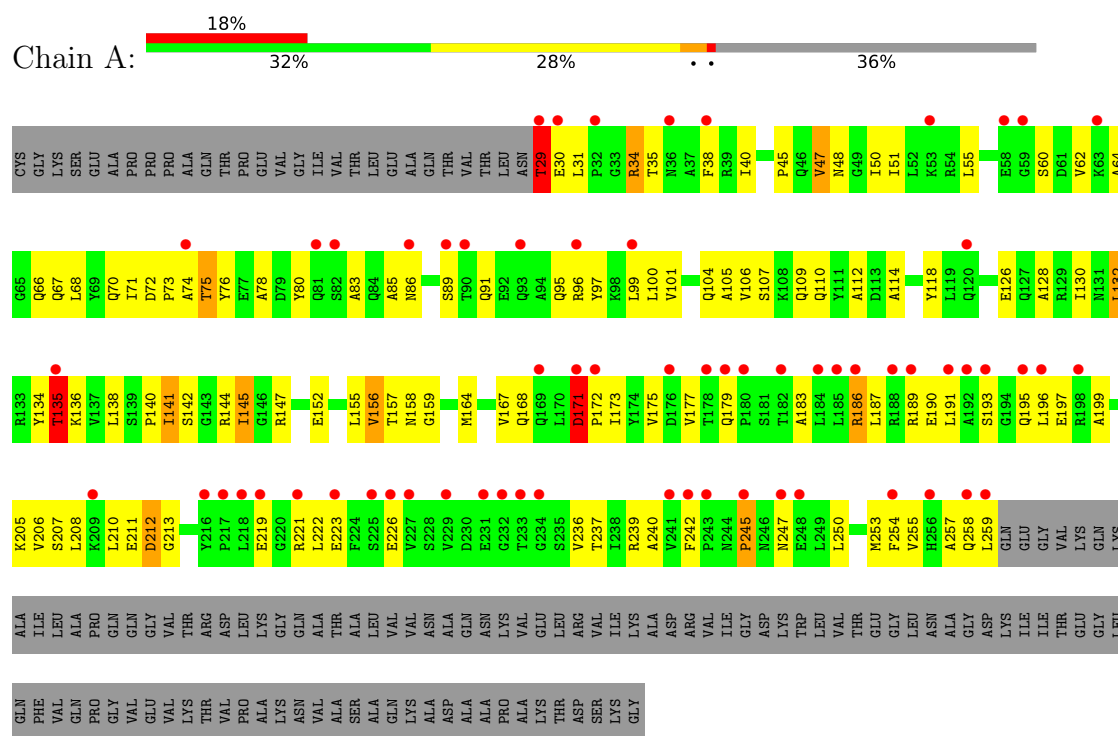


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total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

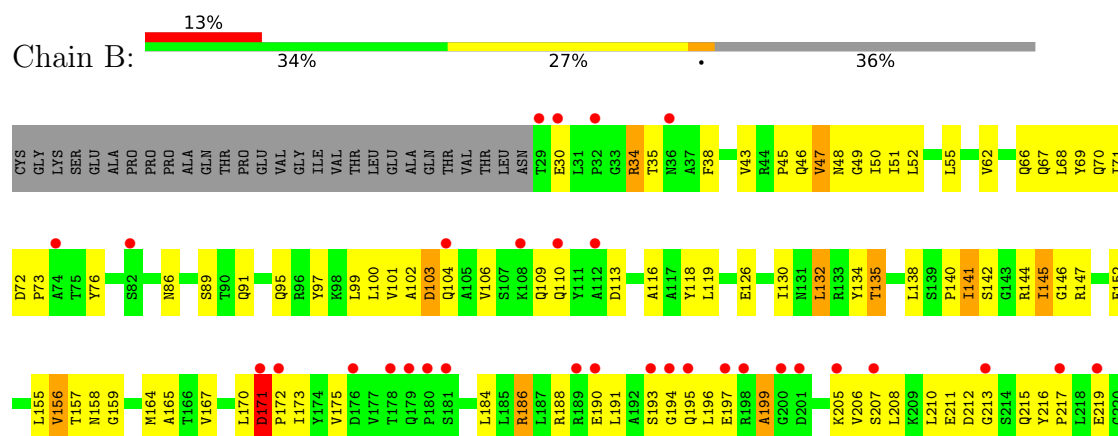
3 Residue-property plots

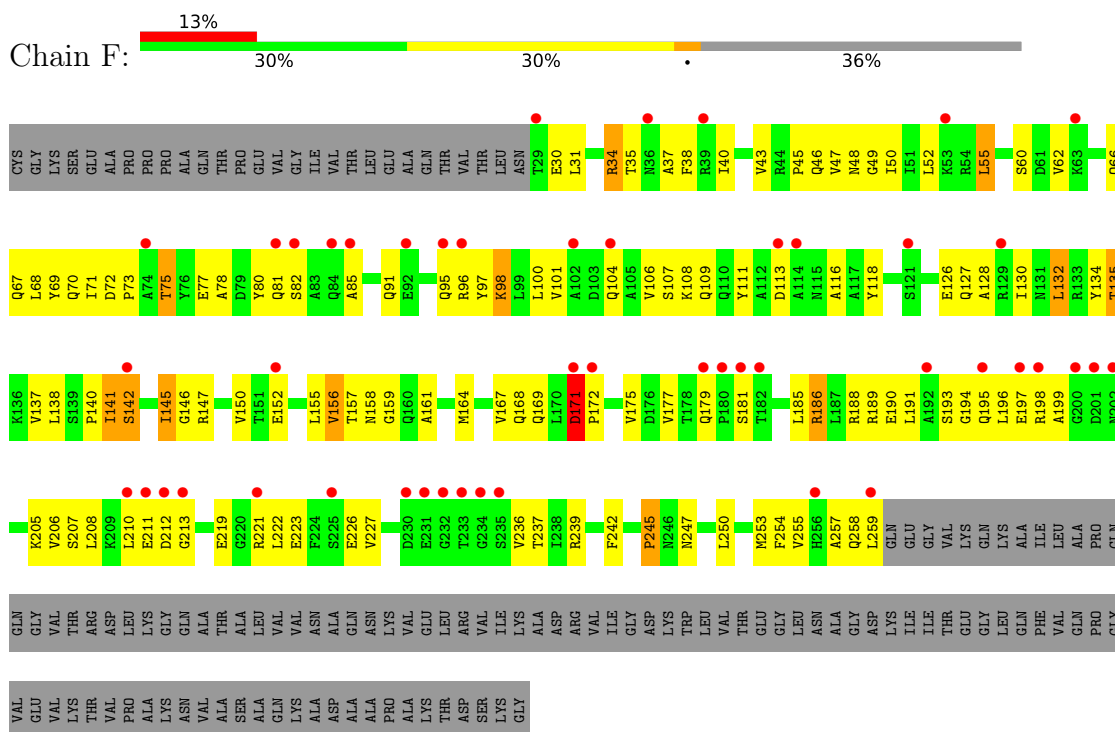
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multidrug resistance protein mexA



• Molecule 1: Multidrug resistance protein mexA





Chain G:

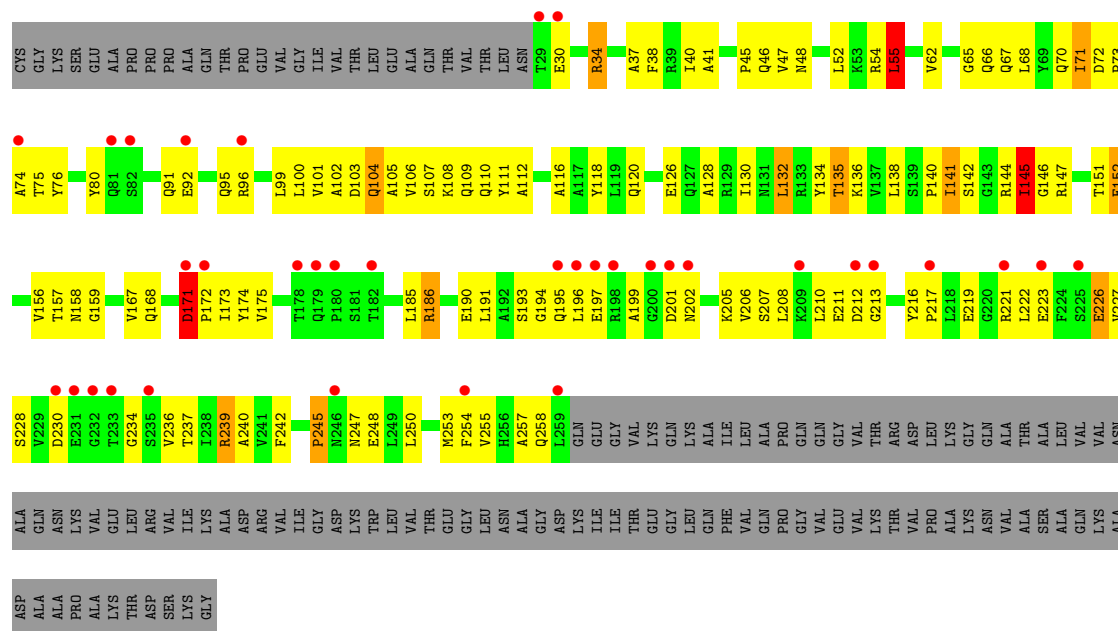
17% 33% 27% 36%

CYS GLY LYS SER GLU PRO ALA THR GLN THR VAL GLU VAL GLY THR VAL THR LEU ASN CYS E30 L31 P32 G33 R34 T35 F38 R39 L40 V43 R44 P45 Q46 V47 N48 G49 T50 L51 L52 R53 R54 L55 F56 R57 E58 G59 S60 D61 L62

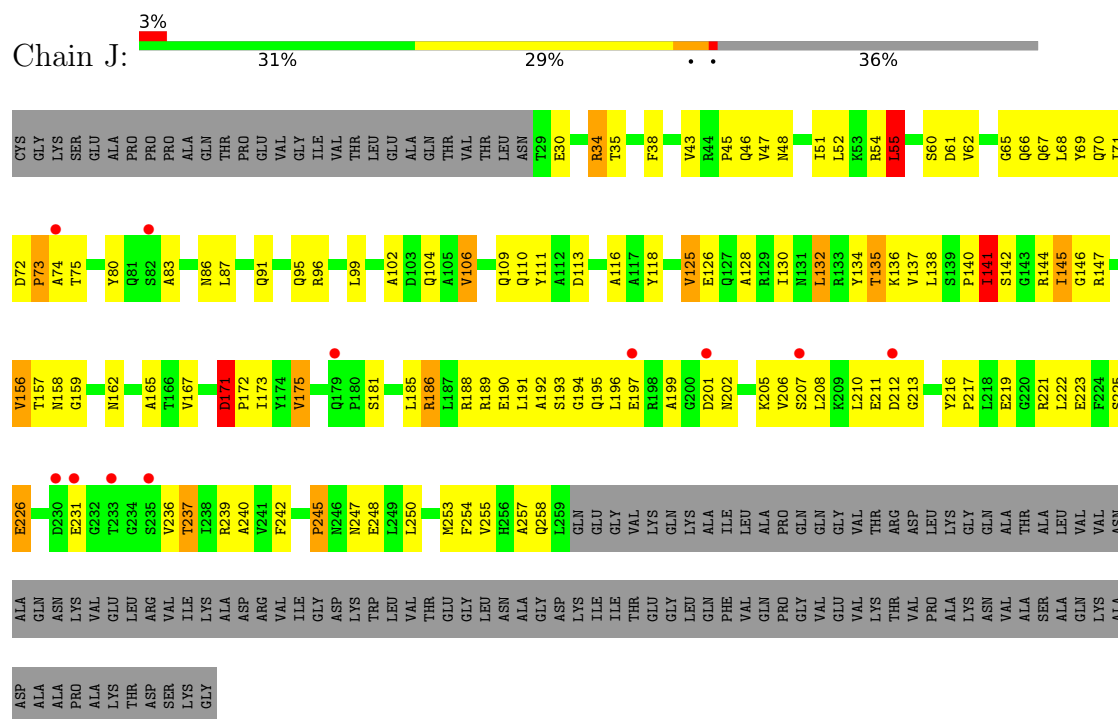
Chain H:

Amino Acid	Percentage
Lys	31%
Val	31%
Ile	31%
Thr	31%
Arg	31%
Ser	31%
Asp	31%
Glu	31%
Ala	31%
Pro	31%
Gly	31%
Leu	29%
Val	29%
Ile	29%
Thr	29%
Arg	29%
Ser	29%
Asp	29%
Glu	29%
Ala	29%
Pro	29%
Gly	29%
Lys	9%
Val	9%
Ile	9%
Thr	9%
Arg	9%
Ser	9%
Asp	9%
Glu	9%
Ala	9%
Pro	9%
Gly	9%
Leu	36%
Val	36%
Ile	36%
Thr	36%
Arg	36%
Ser	36%
Asp	36%
Glu	36%
Ala	36%
Pro	36%
Gly	36%

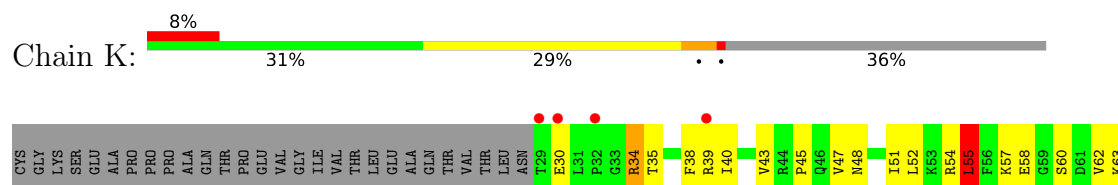
Chain I:

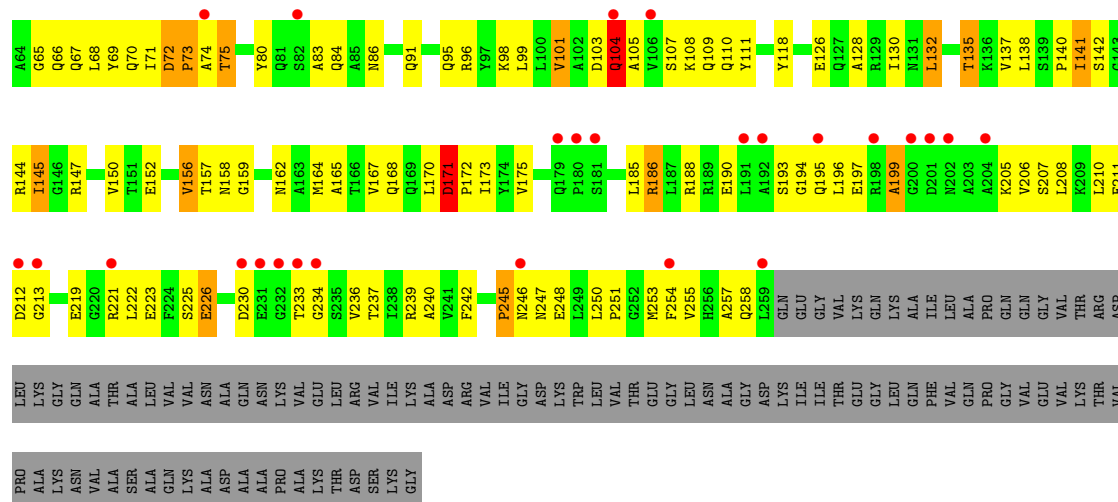


• Molecule 1: Multidrug resistance protein mexA

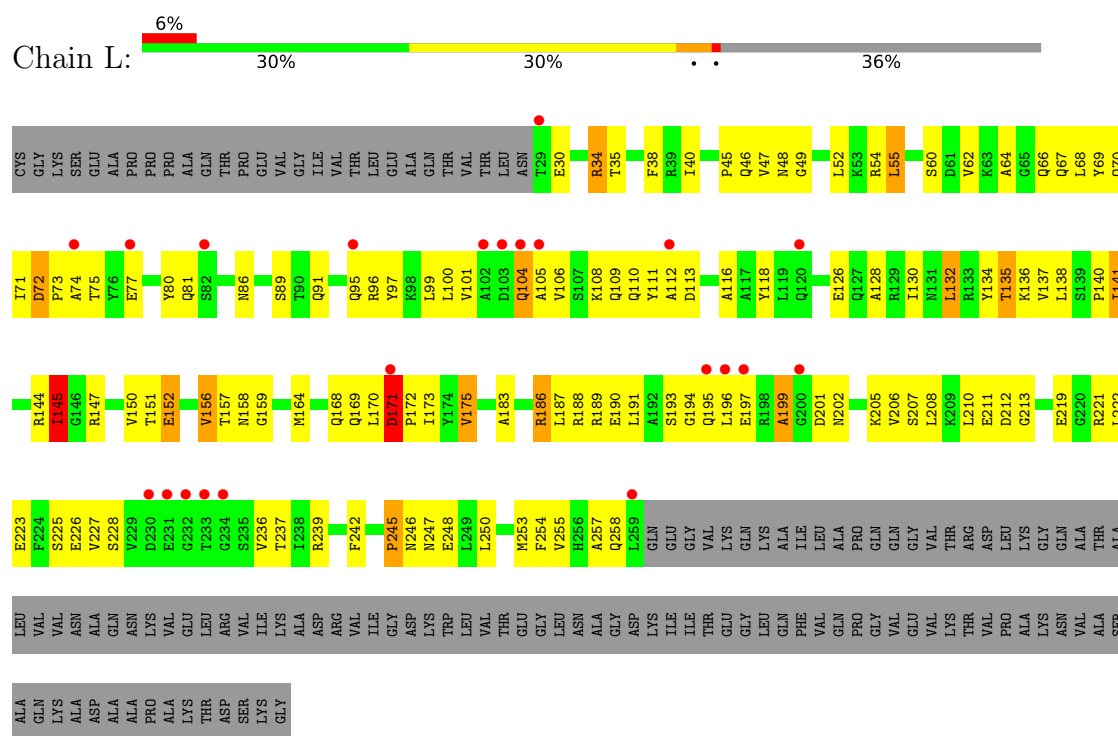


• Molecule 1: Multidrug resistance protein mexA

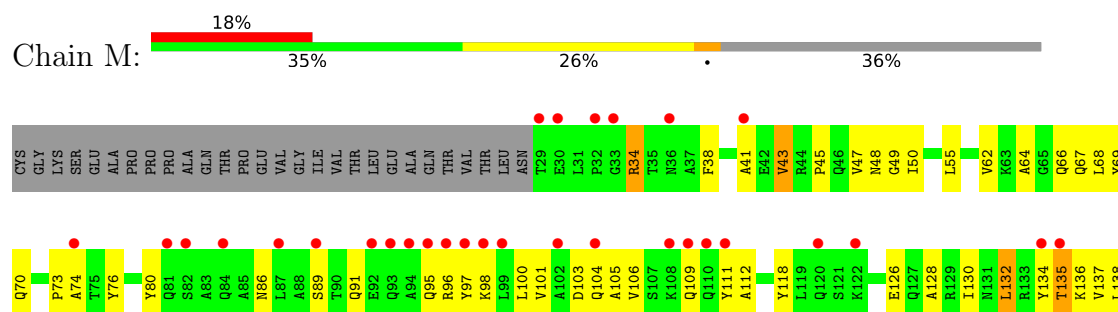




• Molecule 1: Multidrug resistance protein mexA



• Molecule 1: Multidrug resistance protein mexA



Lys	Thr	E211	Thr	S139
Thr	Arg	E212	Arg	P140
Val	Asp	G213	Asp	I141
Pro	Leu		Leu	G142
Ala		E219		S143
Lys	Gly	G220	Gly	R144
Asn	Gln	R221	Gln	I145
Val	Ala	L222	Ala	G146
Ala	Thr	E223	Thr	R147
Ser	Ala	F224	Ala	
Ala	Leu	S225	Leu	T151
Gln	Val	E226	Val	E152
Lys	Val	V227	Val	
Ala	Asn	S228	Asn	L155
Ala	Ala	V229	Ala	V156
Ala	Gln	D230	Gln	T157
Ala	Asn	E231	Asn	N158
Pro	Lys	G232	Lys	G159
Ala	Val	T233	Val	
Lys	Glu	G234	Glu	A165
Thr	Leu	S235	Leu	T166
Asp	Arg	V236	Arg	V167
Ser	Val	T237	Val	
Lys	Ile	L238	Ile	L170
Lys	Lys	R239	Lys	D171
Ala	Ala	A240	Ala	P172
Ala	Asp	V241	Asp	I173
Arg	Arg	F242	Arg	Y174
Val	Val		Val	V175
Ile	Ile	P245	Ile	
Gly	Gly	N246	Gly	T178
Asp	Asp	N247	Asp	Q179
Lys	Lys	E248	Lys	P180
Thr	Thr	L249	Thr	S181
Leu	Leu	L250	Leu	T182
Val	Val	P251	Val	A183
Thr	Thr	G252	Thr	
Glu	Glu	M253	Glu	R186
Gly	Gly	V254	Gly	L187
Leu	Leu	V255	Leu	R188
Asn	Asn	H256	Asn	R189
Ala	Ala	A257	Ala	E190
Gly	Gly	L258	Gly	
Asp	Asp	Q259	Asp	S193
Lys	Lys	Gln	Lys	G194
Ile	Ile	Glu	Ile	Q195
Ile	Ile	Gly	Ile	L196
Thr	Thr	Val	Thr	E197
Glu	Glu	Lys	Glu	R198
Gly	Gly	Gln	Gly	A199
Leu	Leu	Lys	Leu	G200
Ala	Ala	D201	Ala	D201
Ala	Ala	Ile	Ala	N202
Val	Val	Leu	Val	
Gln	Gln	Ala	Gln	K205
Pro	Pro	Pro	Pro	V206
Gly	Gly	Gln	Gly	S207
Val	Val	Gln	Val	L208
Glu	Glu	Gly	Glu	
Val	Val	Val	Val	K209
				L210

4 Data and refinement statistics

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 95.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (95.00-3.00) 98.9 (95.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.268 , 0.278	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 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: GOL, 3GR

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	0.73	1/1795 (0.1%)	0.99	8/2434 (0.3%)
1	B	0.48	0/1795	1.05	8/2434 (0.3%)
1	C	0.51	0/1795	1.03	9/2434 (0.4%)
1	D	0.53	1/1795 (0.1%)	1.12	13/2434 (0.5%)
1	E	0.59	0/1795	1.12	10/2434 (0.4%)
1	F	0.48	0/1795	1.06	9/2434 (0.4%)
1	G	0.45	0/1795	1.02	6/2434 (0.2%)
1	H	0.58	0/1795	1.14	11/2434 (0.5%)
1	I	0.61	0/1795	1.12	9/2434 (0.4%)
1	J	0.74	0/1795	1.19	11/2434 (0.5%)
1	K	0.66	0/1795	1.16	13/2434 (0.5%)
1	L	0.61	0/1795	1.15	13/2434 (0.5%)
1	M	0.48	0/1795	1.06	9/2434 (0.4%)
All	All	0.58	2/23335 (0.0%)	1.09	129/31642 (0.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	C-N	-25.67	1.00	1.33
1	D	164	MET	SD-CE	-5.75	1.65	1.79

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	171	ASP	CA-C-N	-12.84	106.19	119.93
1	J	171	ASP	C-N-CA	-12.84	106.19	119.93
1	H	171	ASP	CA-C-N	-12.34	106.72	119.93
1	H	171	ASP	C-N-CA	-12.34	106.72	119.93
1	E	171	ASP	CA-C-N	-11.51	107.61	119.93

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

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	118	1
1	B	1771	0	1775	110	0
1	C	1771	0	1775	104	0
1	D	1771	0	1775	119	1
1	E	1771	0	1775	107	0
1	F	1771	0	1775	113	0
1	G	1771	0	1775	123	0
1	H	1771	0	1775	118	0
1	I	1771	0	1775	121	0
1	J	1771	0	1775	116	0
1	K	1771	0	1775	125	0
1	L	1771	0	1775	134	0
1	M	1771	0	1775	112	0
2	A	6	0	8	5	0
2	B	6	0	5	3	0
2	J	6	0	5	6	0
2	M	6	0	5	3	0
3	C	6	0	5	2	0
3	D	6	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1440	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 31.

The worst 5 of 1440 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%)	30	65
1	B	229/360 (64%)	203 (89%)	24 (10%)	2 (1%)	14	48
1	C	229/360 (64%)	209 (91%)	18 (8%)	2 (1%)	14	48
1	D	229/360 (64%)	200 (87%)	24 (10%)	5 (2%)	5	26
1	E	229/360 (64%)	211 (92%)	15 (7%)	3 (1%)	9	38
1	F	229/360 (64%)	209 (91%)	17 (7%)	3 (1%)	9	38
1	G	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	H	229/360 (64%)	205 (90%)	19 (8%)	5 (2%)	5	26
1	I	229/360 (64%)	210 (92%)	16 (7%)	3 (1%)	9	38
1	J	229/360 (64%)	208 (91%)	17 (7%)	4 (2%)	7	32
1	K	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	L	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	7	32
1	M	229/360 (64%)	204 (89%)	22 (10%)	3 (1%)	9	38
All	All	2977/4680 (64%)	2681 (90%)	253 (8%)	43 (1%)	9	36

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 ⓘ

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%)	173 (93%)	13 (7%)	14	44
1	B	186/287 (65%)	174 (94%)	12 (6%)	15	47
1	C	186/287 (65%)	174 (94%)	12 (6%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	186/287 (65%)	171 (92%)	15 (8%)	11	38
1	E	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	F	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	G	186/287 (65%)	170 (91%)	16 (9%)	10	36
1	H	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	I	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	J	186/287 (65%)	169 (91%)	17 (9%)	9	33
1	K	186/287 (65%)	170 (91%)	16 (9%)	10	36
1	L	186/287 (65%)	173 (93%)	13 (7%)	14	44
1	M	186/287 (65%)	177 (95%)	9 (5%)	23	57
All	All	2418/3731 (65%)	2235 (92%)	183 (8%)	12	41

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	34	ARG
1	J	226	GLU
1	I	104	GLN
1	J	55	LEU
1	K	104	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	104	GLN
1	K	215	GLN
1	M	70	GLN
1	E	202	ASN
1	E	179	GLN

5.3.3 RNA ⓘ

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

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	GOL	A	361	-	-	0/4/4/4	-
3	3GR	I	361	-	-	1/3/4/4	-
3	3GR	E	361	-	-	1/3/4/4	-
2	GOL	B	361	-	-	0/4/4/4	-
2	GOL	M	361	-	-	0/4/4/4	-
2	GOL	J	361	-	-	0/4/4/4	-
3	3GR	D	361	-	-	1/3/4/4	-
3	3GR	G	361	-	-	1/3/4/4	-
3	3GR	H	361	-	-	1/3/4/4	-
3	3GR	K	361	-	-	1/3/4/4	-
3	3GR	L	361	-	-	1/3/4/4	-
3	3GR	F	361	-	-	1/3/4/4	-
3	3GR	C	361	-	-	1/3/4/4	-

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(°)	Ideal(°)
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 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	GOL	5	0
3	I	361	3GR	4	0
3	E	361	3GR	2	0
2	B	361	GOL	3	0
2	M	361	GOL	3	0
2	J	361	GOL	6	0
3	G	361	3GR	1	0
3	H	361	3GR	2	0
3	K	361	3GR	3	0
3	L	361	3GR	1	0
3	F	361	3GR	4	0
3	C	361	3GR	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%)	1.40	64 (27%) 1 1	29, 93, 132, 143	2 (0%)
1	B	231/360 (64%)	1.10	46 (19%) 3 2	22, 80, 110, 123	2 (0%)
1	C	231/360 (64%)	0.96	36 (15%) 5 3	22, 77, 111, 116	2 (0%)
1	D	231/360 (64%)	0.99	45 (19%) 3 2	16, 82, 109, 123	2 (0%)
1	E	231/360 (64%)	0.59	18 (7%) 19 10	21, 61, 95, 111	2 (0%)
1	F	231/360 (64%)	1.25	48 (20%) 2 2	31, 80, 106, 111	2 (0%)
1	G	231/360 (64%)	1.39	62 (26%) 1 1	31, 86, 118, 126	2 (0%)
1	H	231/360 (64%)	0.88	33 (14%) 6 3	24, 64, 98, 109	2 (0%)
1	I	231/360 (64%)	0.79	35 (15%) 5 3	17, 62, 96, 109	2 (0%)
1	J	231/360 (64%)	0.33	11 (4%) 35 19	8, 48, 84, 100	2 (0%)
1	K	231/360 (64%)	0.73	30 (12%) 7 4	11, 59, 92, 107	2 (0%)
1	L	231/360 (64%)	0.59	22 (9%) 14 7	14, 63, 102, 115	2 (0%)
1	M	231/360 (64%)	1.48	63 (27%) 1 1	25, 93, 117, 130	2 (0%)
All	All	3003/4680 (64%)	0.96	513 (17%) 4 3	8, 75, 114, 143	26 (0%)

The worst 5 of 513 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	82	SER	10.2
1	C	82	SER	10.2
1	A	82	SER	9.9
1	B	82	SER	8.9
1	D	82	SER	8.9

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 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(Å ²)	Q<0.9
2	GOL	A	361	6/6	0.42	0.40	97,98,99,102	0
3	3GR	F	361	6/6	0.48	0.41	99,100,101,103	0
2	GOL	B	361	6/6	0.53	0.45	95,96,96,96	0
3	3GR	E	361	6/6	0.58	0.51	93,95,98,102	0
3	3GR	G	361	6/6	0.59	0.41	103,104,105,106	0
3	3GR	H	361	6/6	0.60	0.41	87,88,89,90	0
2	GOL	M	361	6/6	0.67	0.33	99,100,101,101	0
3	3GR	D	361	6/6	0.67	0.52	93,93,94,95	0
3	3GR	C	361	6/6	0.68	0.46	100,100,101,102	0
3	3GR	K	361	6/6	0.71	0.43	79,80,83,84	0
3	3GR	I	361	6/6	0.76	0.35	87,87,88,88	0
2	GOL	J	361	6/6	0.76	0.39	92,94,94,96	0
3	3GR	L	361	6/6	0.77	0.36	81,82,83,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.