



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 05:35 PM BST

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

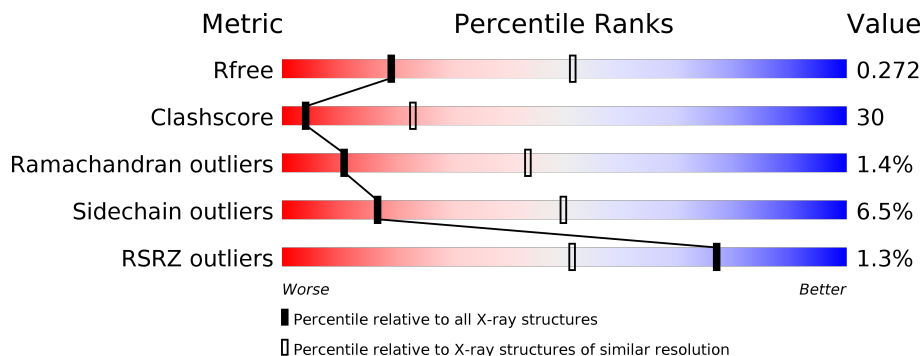
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on 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	 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%
1	F	360	 % 33% 28% 36%

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Mol	Chain	Length	Quality of chain
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	-
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.

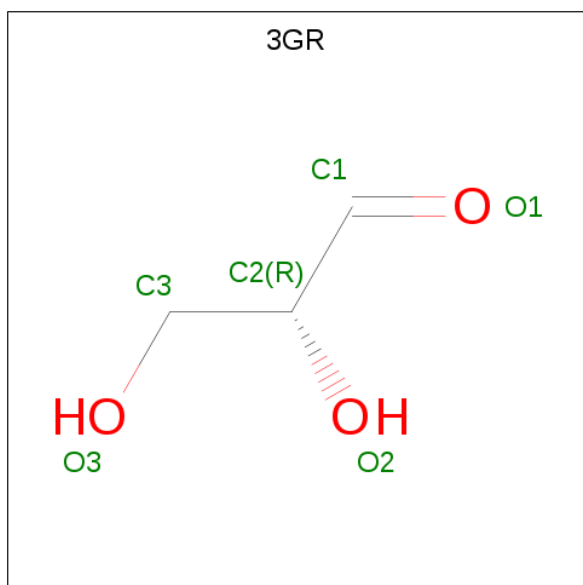
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1771	1101	319	349	2	0	0	0
1	B	231	1771	1101	319	349	2	0	0	0
1	C	231	1771	1101	319	349	2	0	0	0
1	D	231	1771	1101	319	349	2	0	0	0
1	E	231	1771	1101	319	349	2	0	0	0
1	F	231	1771	1101	319	349	2	0	0	0
1	G	231	1771	1101	319	349	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: 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 (three-letter code: 3GR) (formula: $C_3H_6O_3$).

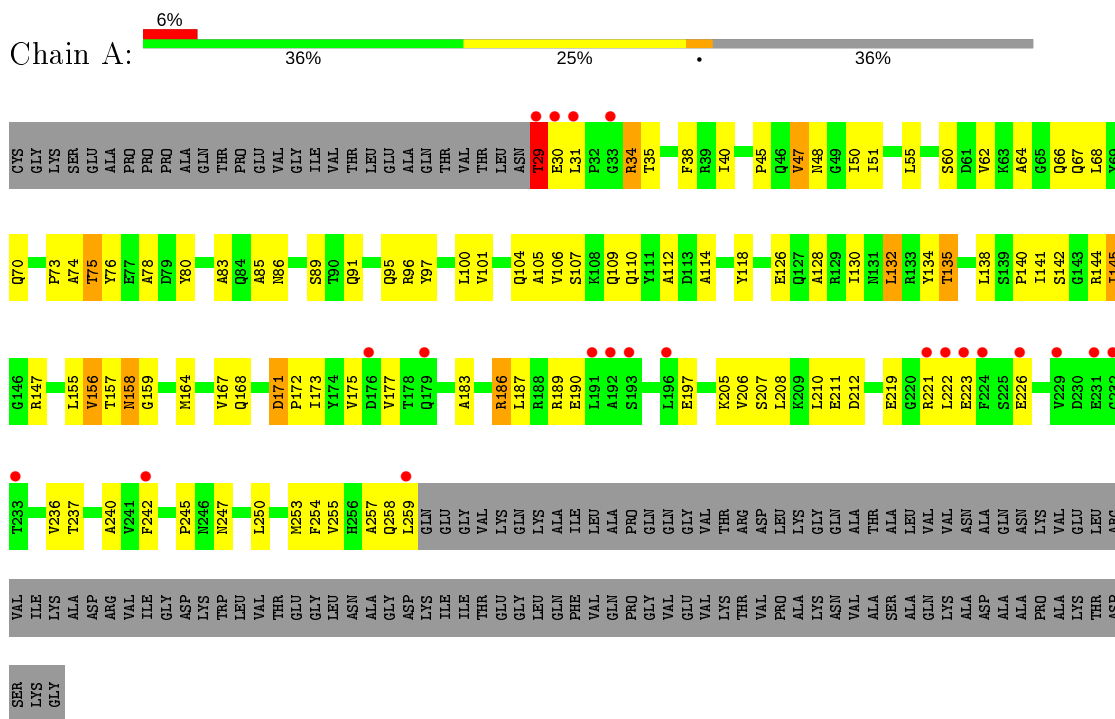


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	I	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0

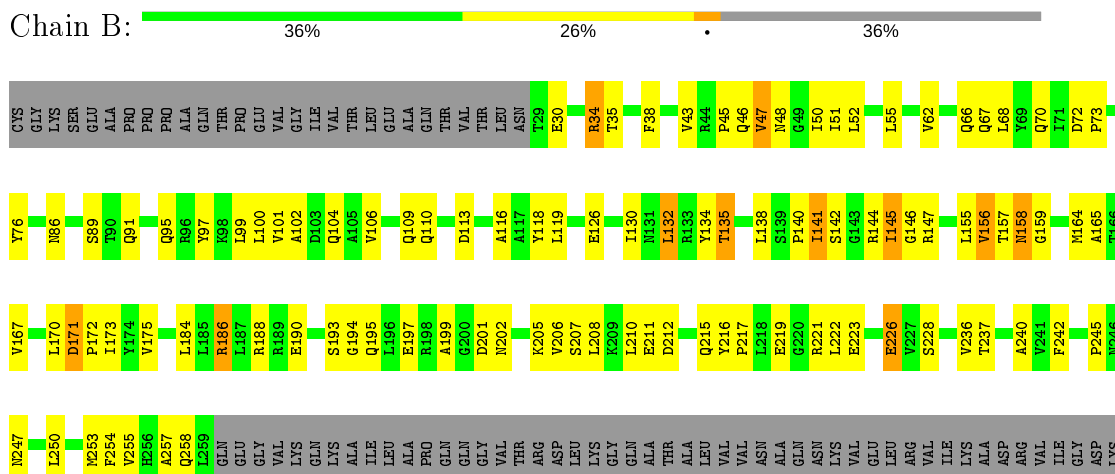
3 Residue-property plots [i](#)

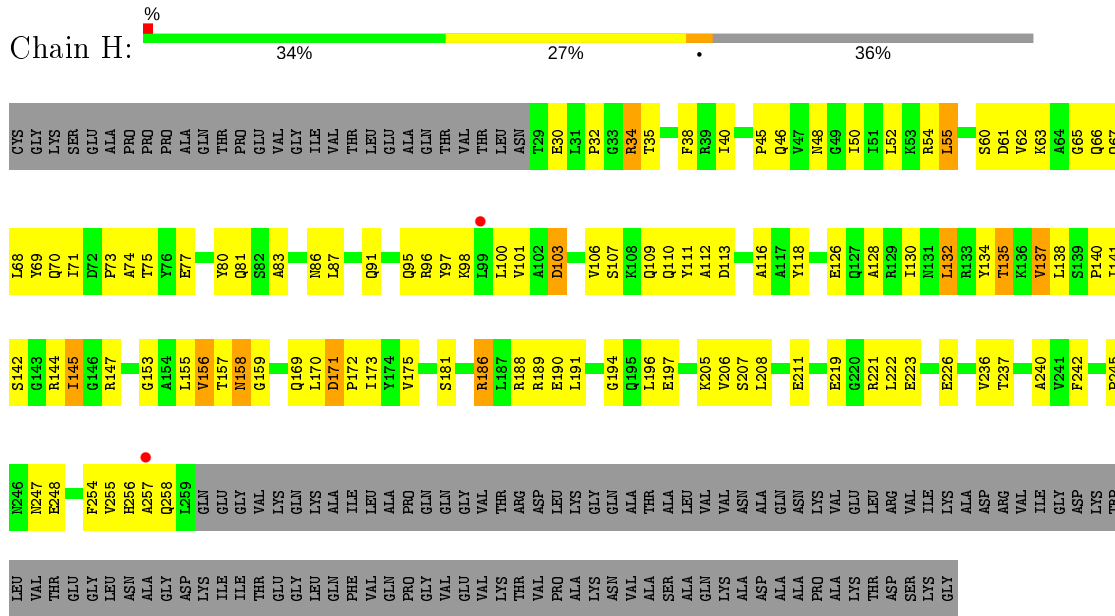
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

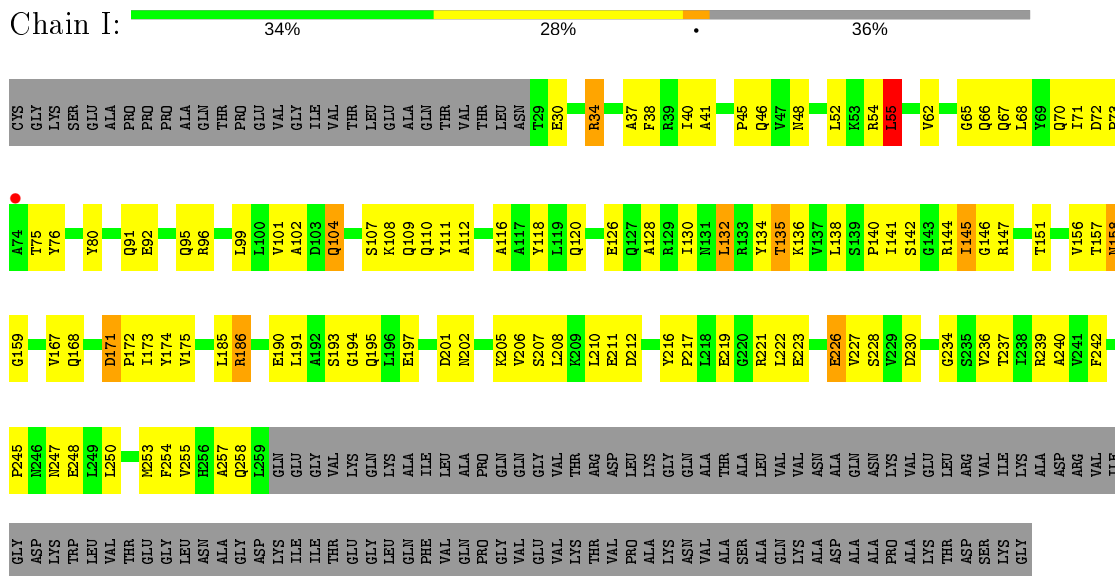


- Molecule 1: Multidrug resistance protein mexA

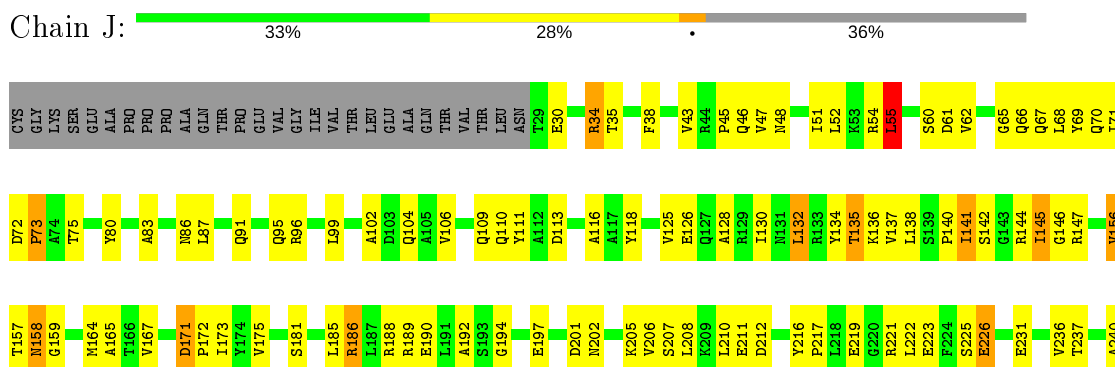




- Molecule 1: Multidrug resistance protein mexA



- Molecule 1: Multidrug resistance protein mexA



Y76	A165	L250	LEU
Y80	T166	F251	VAL
N86	V167	G252	THR
S89	L170	M253	GLU
F90	D171	F254	GLY
Q91	F172	Y255	LEU
Q95	I173	H256	ASN
R96	V174	A257	ALA
Y97	V175	Q258	GLY
K98	Q179	L259	ASP
L99	A183	GLN	LYS
L100	R186	GLU	ILE
V101	L187	GLY	THR
D103	E190	VAL	GLU
Q104	S193	GLN	LYS
A105	Q194	PRO	PRO
V106	Q195	VAL	VAL
Q109	Q196	GLN	GLY
G110	L198	GLY	GLU
Y111	E197	VAL	VAL
A112	R199	LYS	LYS
Y118	A199	THR	THR
E126	K205	VAL	VAL
Q127	V206	PRO	PRO
A128	S207	ALA	ALA
R129	S207	LYS	LYS
I130	L208	ASN	ASN
N131	K209	VAL	VAL
L132	L210	ALA	ALA
R133	E211	THR	THR
Y134	D212	ALA	ALA
T135	E219	LEU	GLN
K136	G220	VAL	LYS
V137	R221	ALA	ALA
L138	L222	ASP	ASP
S139	E223	ALA	ALA
P140	F224	ASN	ALA
I141	S225	LYS	ALA
S142	E226	VAL	LYS
G143	V227	THR	THR
I144	V236	ASP	SER
I145	T237	ARG	LYS
G146	A240	VAL	GLY
R147	V241	ILE	ILE
T151	F242	LYS	LYS
L155	P245	ALA	ALA
V156	R246	ASP	ASP
T157	R247	ARG	ARG
N158	E248	VAL	VAL
G159	L249	LYS	LYS
		TRP	TRP

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
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.262 , 0.272	Depositor DCC
R_{free} test set	9310 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	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

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	F	189	ARG
1	H	103	ASP
1	L	186	ARG
1	G	34	ARG
1	G	145	ILE

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

Mol	Chain	Res	Type
1	G	84	GLN
1	H	95	GLN
1	M	70	GLN
1	G	110	GLN
1	G	169	GLN

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	E	361	-	4,5,5	6.06	2 (50%)	4,5,5	14.71	1 (25%)
2	GOL	A	361	-	5,5,5	0.23	0	5,5,5	0.46	0
3	3GR	I	361	-	4,5,5	6.06	2 (50%)	4,5,5	14.71	1 (25%)
2	GOL	J	361	1	5,5,5	4.76	1 (20%)	5,5,5	4.22	1 (20%)
3	3GR	C	361	-	4,5,5	6.06	2 (50%)	4,5,5	14.73	1 (25%)
3	3GR	G	361	-	4,5,5	6.07	2 (50%)	4,5,5	14.71	1 (25%)
3	3GR	H	361	-	4,5,5	6.06	2 (50%)	4,5,5	14.72	1 (25%)
2	GOL	M	361	1	5,5,5	4.76	1 (20%)	5,5,5	4.22	1 (20%)
3	3GR	L	361	-	4,5,5	6.06	2 (50%)	4,5,5	14.72	1 (25%)
3	3GR	D	361	-	4,5,5	6.05	2 (50%)	4,5,5	14.72	1 (25%)
3	3GR	F	361	-	4,5,5	6.05	2 (50%)	4,5,5	14.71	1 (25%)
2	GOL	B	361	-	5,5,5	4.76	1 (20%)	5,5,5	4.21	1 (20%)
3	3GR	K	361	-	4,5,5	6.05	2 (50%)	4,5,5	14.72	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
3	3GR	E	361	-	-	1/3/4/4	-
2	GOL	A	361	-	-	0/4/4/4	-
3	3GR	I	361	-	-	1/3/4/4	-
2	GOL	J	361	1	-	0/4/4/4	-
3	3GR	C	361	-	-	1/3/4/4	-
3	3GR	G	361	-	-	1/3/4/4	-
3	3GR	H	361	-	-	1/3/4/4	-
2	GOL	M	361	1	-	0/4/4/4	-
3	3GR	L	361	-	-	1/3/4/4	-
3	3GR	D	361	-	-	1/3/4/4	-
3	3GR	F	361	-	-	1/3/4/4	-
2	GOL	B	361	-	-	0/4/4/4	-
3	3GR	K	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	-10.62	0.97	1.42
3	I	361	3GR	O3-C3	-10.62	0.97	1.42
3	H	361	3GR	O3-C3	-10.61	0.97	1.42
3	L	361	3GR	O3-C3	-10.61	0.97	1.42
2	M	361	GOL	O3-C3	-10.61	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	29.44	155.34	112.40
3	K	361	3GR	O3-C3-C2	29.43	155.32	112.40
3	D	361	3GR	O3-C3-C2	29.43	155.32	112.40
3	H	361	3GR	O3-C3-C2	29.43	155.32	112.40
3	L	361	3GR	O3-C3-C2	29.42	155.31	112.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	361	3GR	O2-C2-C3-O3
3	I	361	3GR	O2-C2-C3-O3
3	C	361	3GR	O2-C2-C3-O3
3	G	361	3GR	O2-C2-C3-O3
3	H	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	E	361	3GR	2	0
2	A	361	GOL	5	0
3	I	361	3GR	4	0
2	J	361	GOL	5	0
3	C	361	3GR	2	0
3	G	361	3GR	1	0
3	H	361	3GR	2	0
2	M	361	GOL	2	0
3	L	361	3GR	1	0
3	F	361	3GR	4	0
2	B	361	GOL	3	0
3	K	361	3GR	3	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%)	0.09	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	L	361	6/6	0.86	0.35	81,82,83,86	0
3	3GR	I	361	6/6	0.86	0.30	87,87,88,88	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.