



wwPDB EM Map/Model Validation Report ⓘ

Aug 4, 2016 – 06:00 PM EDT

PDB ID : 5LDF
EMDB ID: : EMD-4039
Title : Maltose binding protein genetically fused to dodecameric glutamine synthetase
Authors : Coscia, F.; Petosa, C.; Schoehn, G.
Deposited on : 2016-06-25
Resolution : 6.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

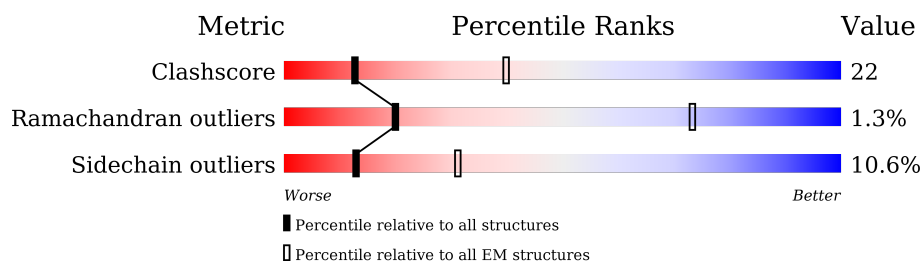
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	466	66% 27% 6% .
1	B	466	67% 26% 6% .
1	C	466	67% 26% 6% .
1	D	466	66% 27% 6% .
1	E	466	67% 26% 6% .
1	F	466	65% 27% 6% .
1	G	466	67% 25% 6% .
1	H	466	67% 26% 6% .
1	I	466	67% 26% 6% .

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Mol	Chain	Length	Quality of chain
1	J	466	 67% 26% 6% .
1	K	466	 67% 26% 6% .
1	L	466	 67% 26% 6% .
2	M	370	 54% 30% 12% .
2	N	370	 53% 31% 12% .
2	O	370	 54% 31% 12% .
2	P	370	 52% 33% 11% .
2	Q	370	 54% 31% 11% .
2	R	370	 54% 31% 11% .
2	S	370	 54% 31% 11% .
2	T	370	 54% 31% 11% .
2	U	370	 53% 32% 11% .
2	V	370	 53% 32% 11% .
2	W	370	 54% 31% 12% .
2	X	370	 54% 31% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 78120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	B	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	C	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	D	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	E	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	F	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	G	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	H	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	I	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	J	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	K	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	L	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	PRO	ALA	conflict	UNP P0A1P7
B	391	PRO	ALA	conflict	UNP P0A1P7
C	391	PRO	ALA	conflict	UNP P0A1P7
D	391	PRO	ALA	conflict	UNP P0A1P7
E	391	PRO	ALA	conflict	UNP P0A1P7
F	391	PRO	ALA	conflict	UNP P0A1P7

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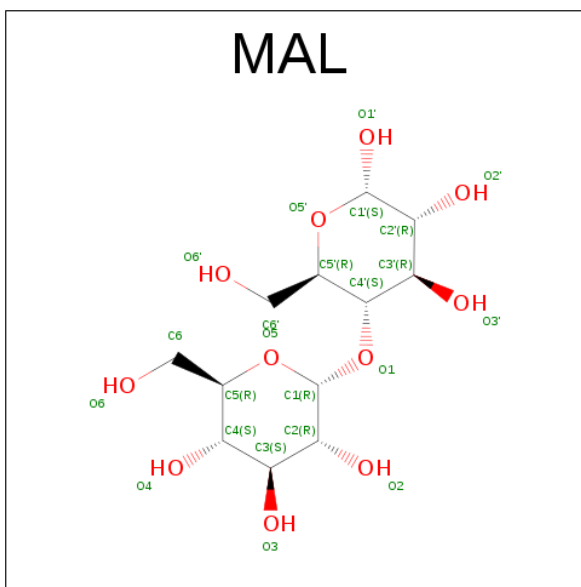
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Chain	Residue	Modelled	Actual	Comment	Reference
G	391	PRO	ALA	conflict	UNP P0A1P7
H	391	PRO	ALA	conflict	UNP P0A1P7
I	391	PRO	ALA	conflict	UNP P0A1P7
J	391	PRO	ALA	conflict	UNP P0A1P7
K	391	PRO	ALA	conflict	UNP P0A1P7
L	391	PRO	ALA	conflict	UNP P0A1P7

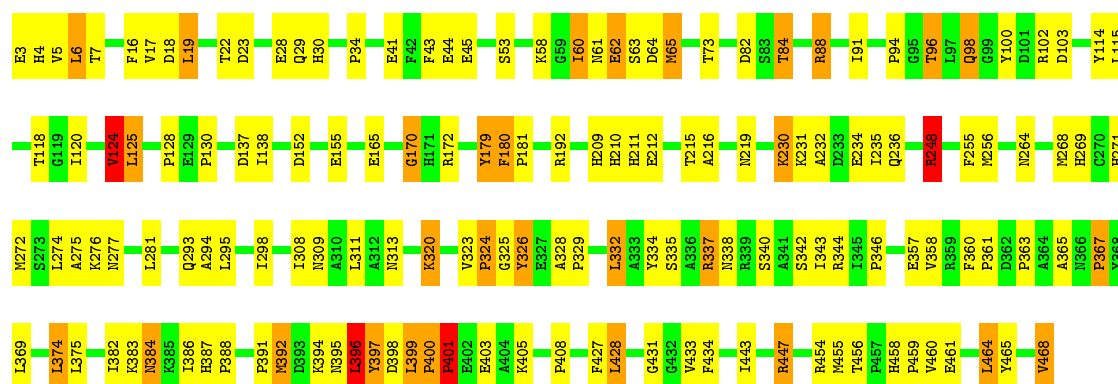
- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	N	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	O	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	P	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	Q	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	R	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	S	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	T	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	U	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	V	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	W	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	X	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).

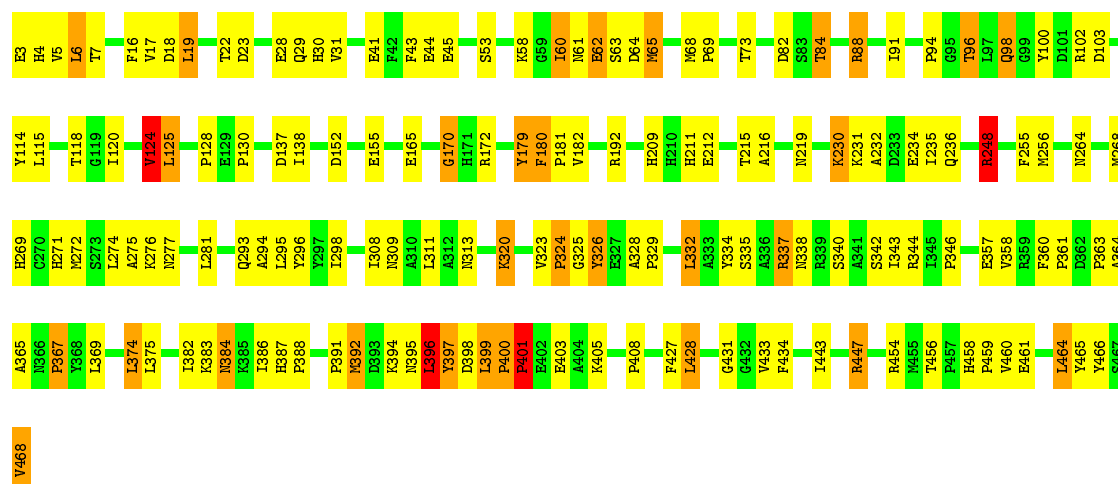


Mol	Chain	Residues	Atoms			AltConf
3	M	1	Total	C	O	0
			23	12	11	
3	N	1	Total	C	O	0
			23	12	11	
3	O	1	Total	C	O	0
			23	12	11	
3	P	1	Total	C	O	0
			23	12	11	
3	Q	1	Total	C	O	0
			23	12	11	
3	R	1	Total	C	O	0
			23	12	11	
3	S	1	Total	C	O	0
			23	12	11	
3	T	1	Total	C	O	0
			23	12	11	
3	U	1	Total	C	O	0
			23	12	11	
3	V	1	Total	C	O	0
			23	12	11	
3	W	1	Total	C	O	0
			23	12	11	
3	X	1	Total	C	O	0
			23	12	11	



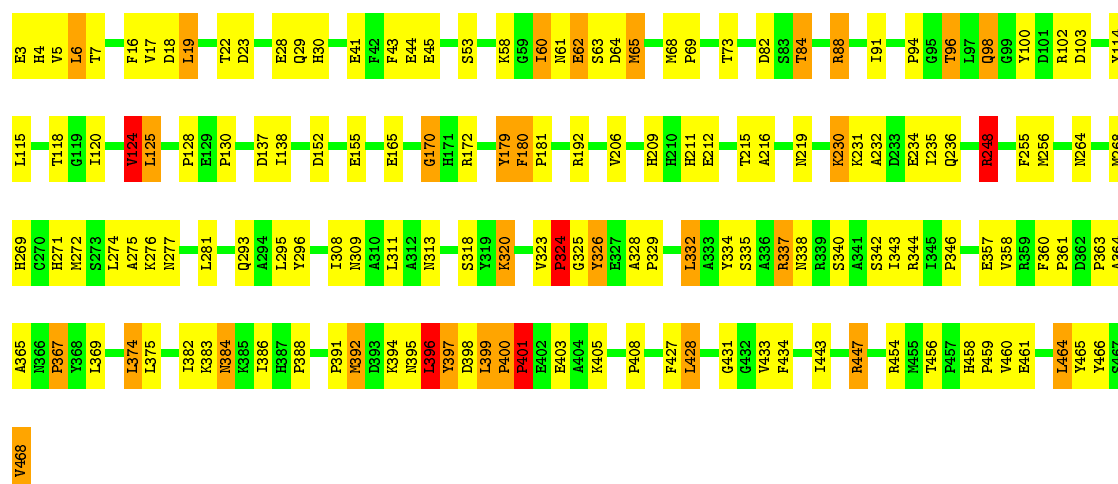
• Molecule 1: Glutamine synthetase

Chain D: 66% 27% 6% •



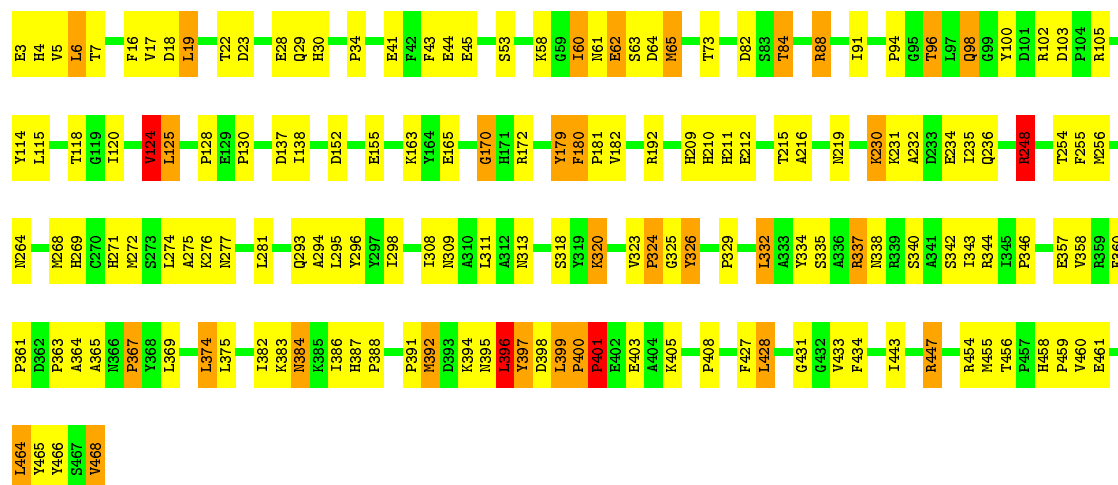
• Molecule 1: Glutamine synthetase

Chain E: 67% 26% 6% •



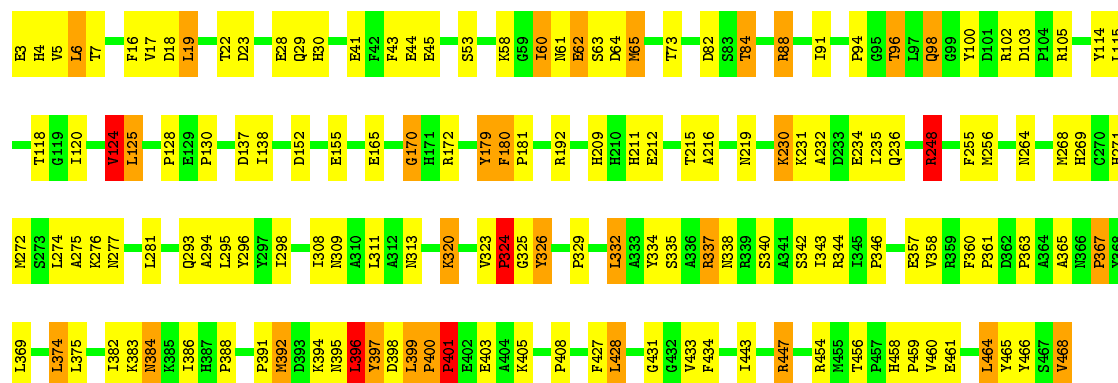
• Molecule 1: Glutamine synthetase

Chain F:  65% 27% 6% •



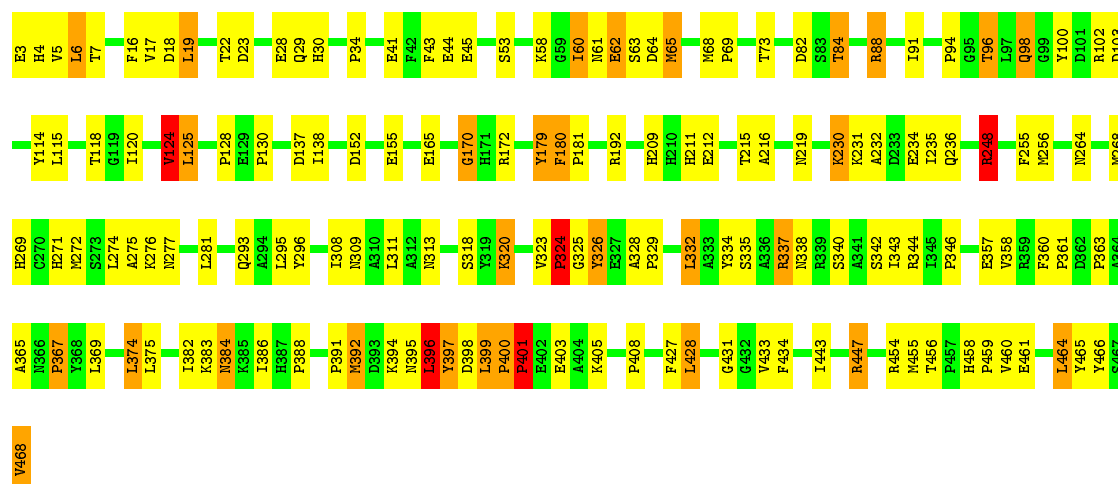
• Molecule 1: Glutamine synthetase

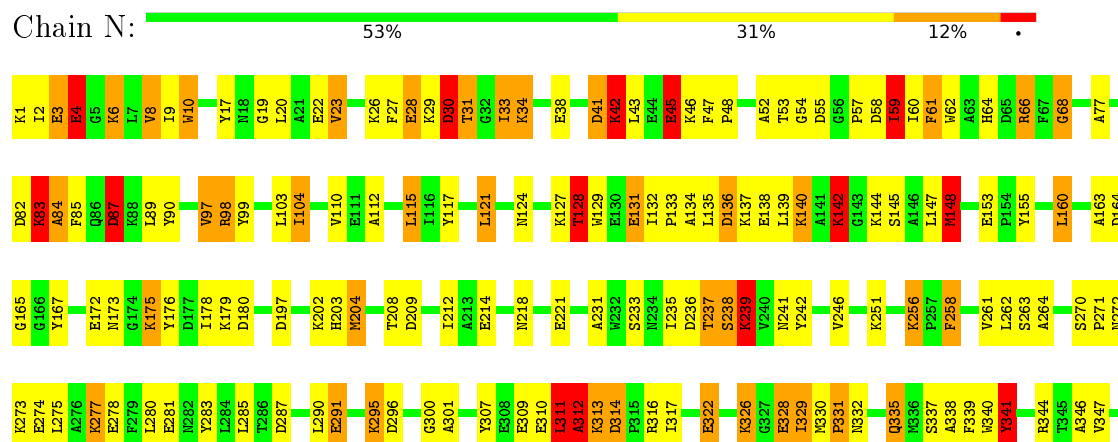
Chain G:  67% 25% 6% •

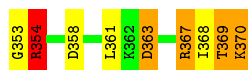


• Molecule 1: Glutamine synthetase

Chain H:  67% 26% 6% •

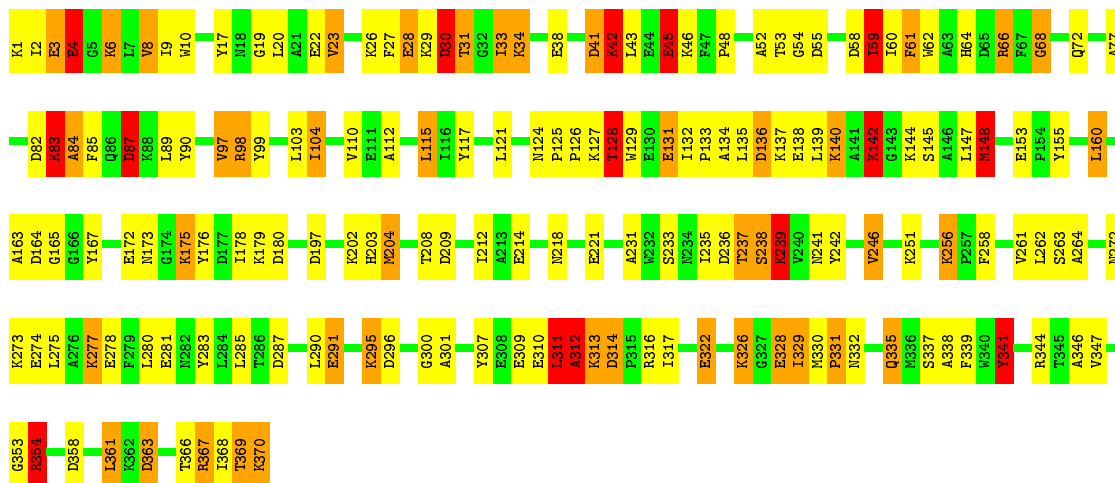






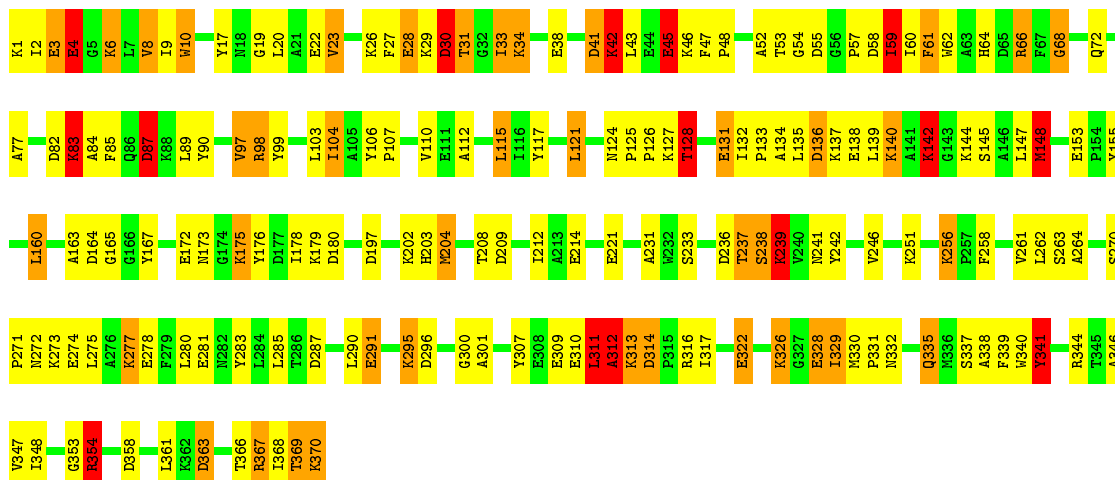
• Molecule 2: Maltose-binding periplasmic protein

Chain O: 54% 31% 12%



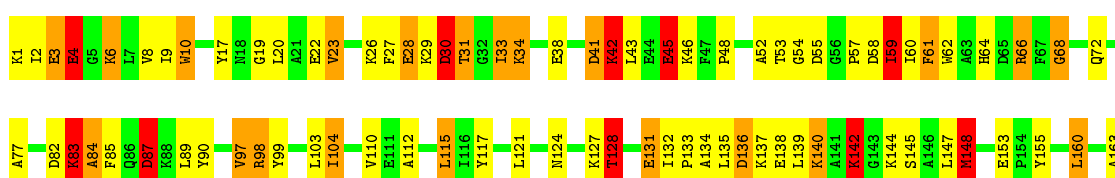
• Molecule 2: Maltose-binding periplasmic protein

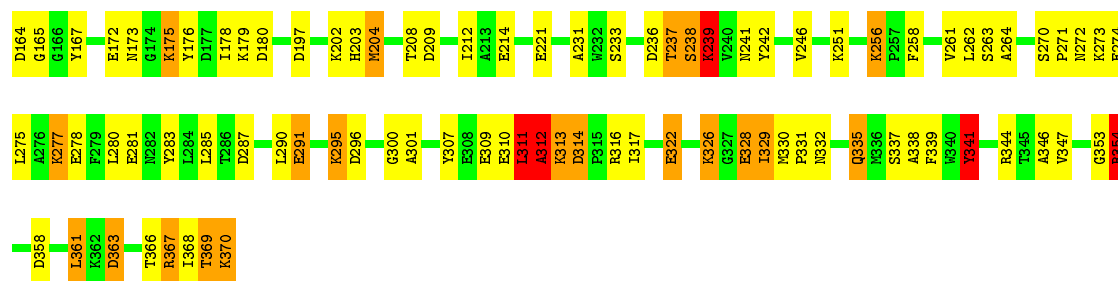
Chain P: 52% 33% 11%



• Molecule 2: Maltose-binding periplasmic protein

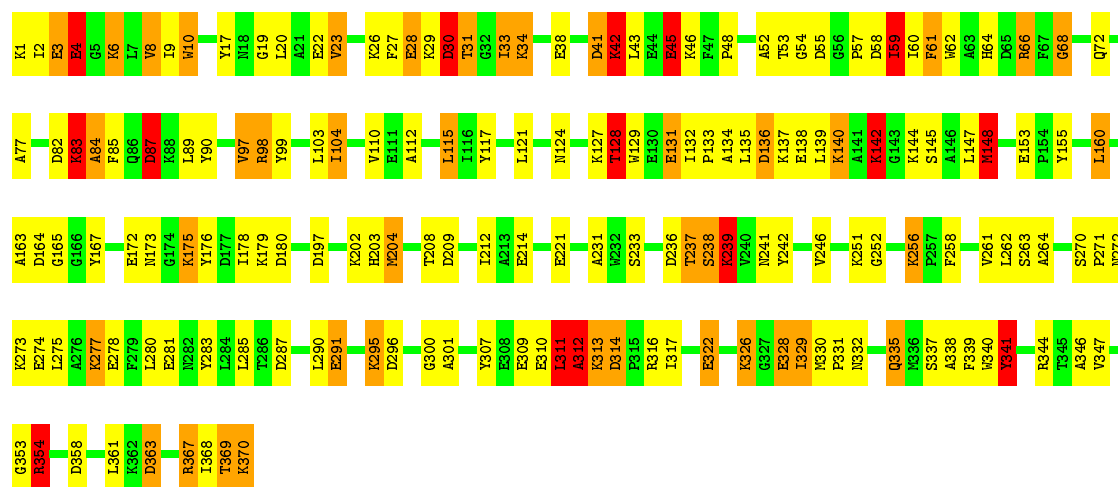
Chain Q: 54% 31% 11%





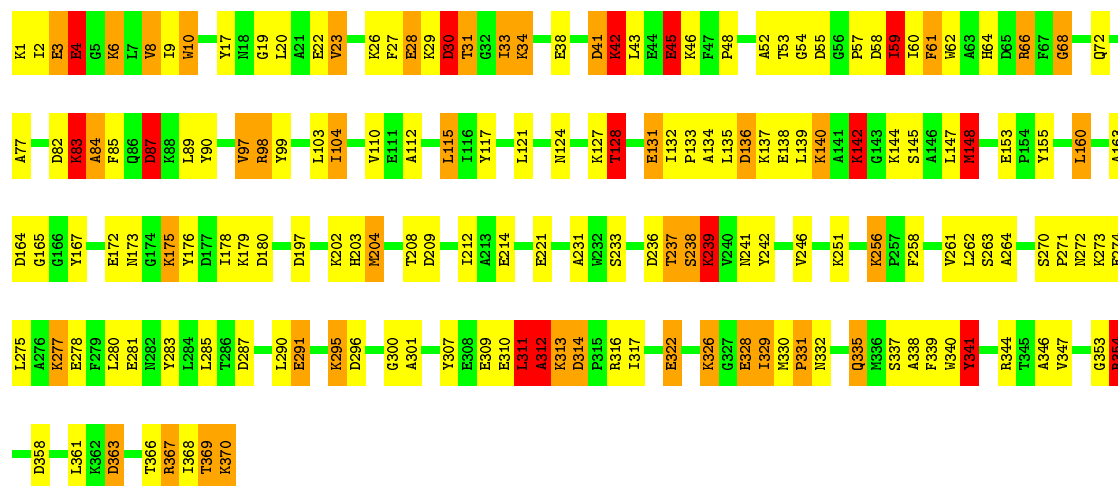
• Molecule 2: Maltose-binding periplasmic protein

Chain R: 54% 31% 11% .



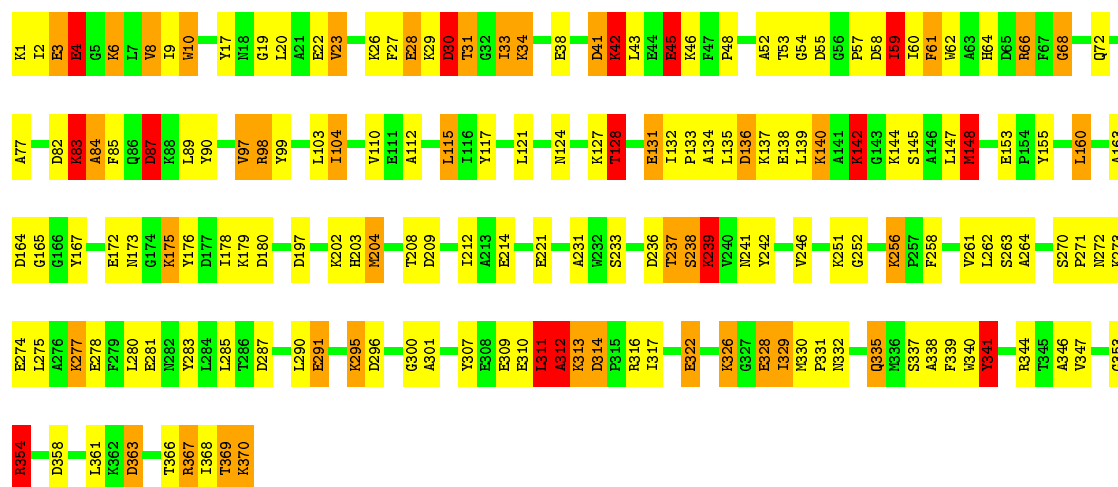
• Molecule 2: Maltose-binding periplasmic protein

Chain S: 54% 31% 11% .



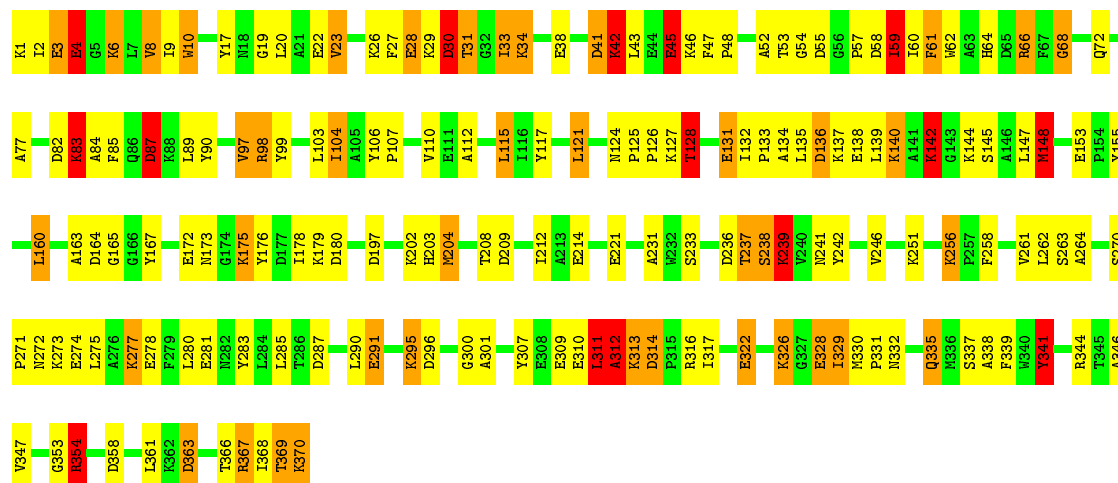
• Molecule 2: Maltose-binding periplasmic protein

Chain T: 54% 31% 11% .



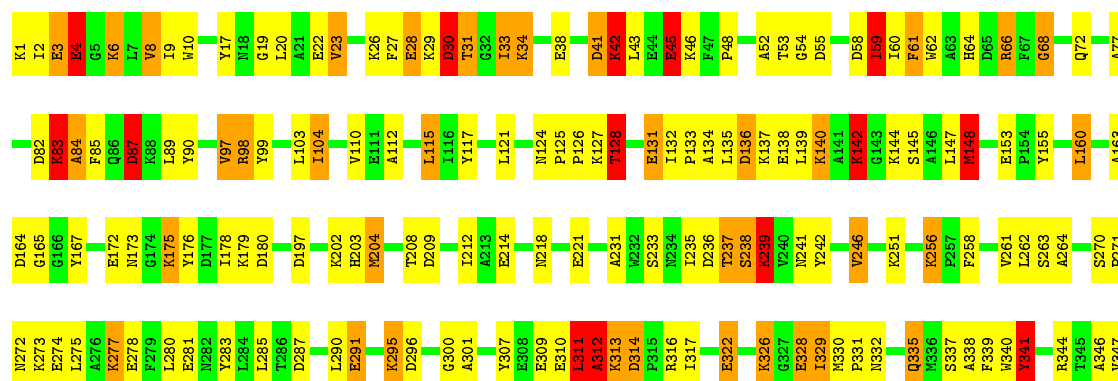
• Molecule 2: Maltose-binding periplasmic protein

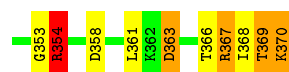
Chain U: 53% 32% 11%



• Molecule 2: Maltose-binding periplasmic protein

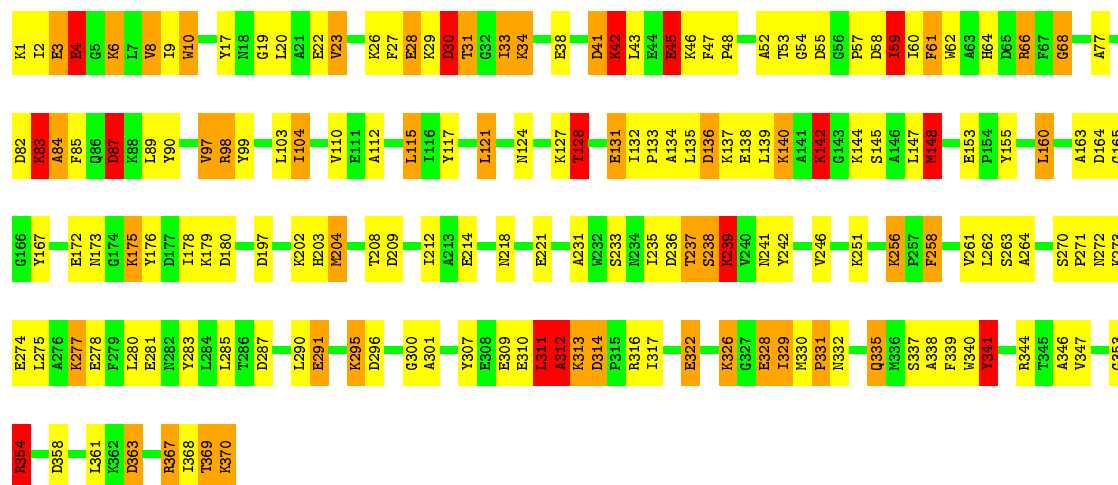
Chain V: 53% 32% 11%





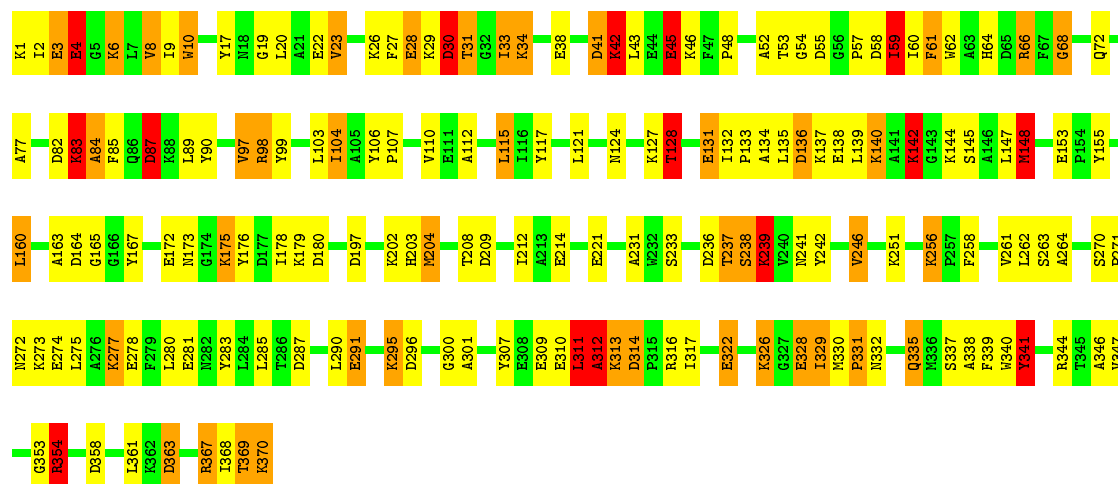
• Molecule 2: Maltose-binding periplasmic protein

Chain W: 54% 31% 12% .



• Molecule 2: Maltose-binding periplasmic protein

Chain X: 54% 31% 12% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAL

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 >2	RMSZ	# Z >2
1	A	0.53	0/3713	0.85	4/5028 (0.1%)
1	B	0.53	0/3713	0.85	4/5028 (0.1%)
1	C	0.53	0/3713	0.85	4/5028 (0.1%)
1	D	0.53	0/3713	0.85	4/5028 (0.1%)
1	E	0.53	0/3713	0.85	4/5028 (0.1%)
1	F	0.53	0/3713	0.85	4/5028 (0.1%)
1	G	0.53	0/3713	0.85	4/5028 (0.1%)
1	H	0.53	0/3713	0.85	4/5028 (0.1%)
1	I	0.53	0/3713	0.85	4/5028 (0.1%)
1	J	0.53	0/3713	0.85	4/5028 (0.1%)
1	K	0.53	0/3713	0.85	4/5028 (0.1%)
1	L	0.53	0/3713	0.85	4/5028 (0.1%)
2	M	1.51	12/2930 (0.4%)	2.43	146/3979 (3.7%)
2	N	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	O	1.51	11/2930 (0.4%)	2.43	147/3979 (3.7%)
2	P	1.51	11/2930 (0.4%)	2.43	145/3979 (3.6%)
2	Q	1.51	11/2930 (0.4%)	2.43	144/3979 (3.6%)
2	R	1.51	13/2930 (0.4%)	2.43	148/3979 (3.7%)
2	S	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	T	1.51	12/2930 (0.4%)	2.43	147/3979 (3.7%)
2	U	1.51	11/2930 (0.4%)	2.43	145/3979 (3.6%)
2	V	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	W	1.51	11/2930 (0.4%)	2.43	146/3979 (3.7%)
2	X	1.51	12/2930 (0.4%)	2.43	145/3979 (3.6%)
All	All	1.08	137/79716 (0.2%)	1.74	1799/108084 (1.7%)

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
2	M	0	2
2	N	0	2
2	O	0	2
2	P	0	2
2	Q	0	2
2	R	0	2
2	S	0	2
2	T	0	2
2	U	0	2
2	V	0	2
2	W	0	2
2	X	0	2
All	All	0	24

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	369	THR	C-N	15.02	1.68	1.34
2	O	369	THR	C-N	14.75	1.68	1.34
2	T	369	THR	C-N	14.75	1.68	1.34
2	P	369	THR	C-N	14.75	1.68	1.34
2	Q	369	THR	C-N	14.74	1.68	1.34

The worst 5 of 1799 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	354	ARG	NE-CZ-NH1	40.58	140.59	120.30
2	N	354	ARG	NE-CZ-NH1	40.56	140.58	120.30
2	S	354	ARG	NE-CZ-NH1	40.55	140.57	120.30
2	R	354	ARG	NE-CZ-NH1	40.53	140.56	120.30
2	T	354	ARG	NE-CZ-NH1	40.52	140.56	120.30

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	312	ALA	Peptide
2	M	354	ARG	Sidechain
2	N	312	ALA	Peptide
2	N	354	ARG	Sidechain
2	O	312	ALA	Peptide

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	3626	0	3531	193	0
1	B	3626	0	3531	187	0
1	C	3626	0	3531	183	0
1	D	3626	0	3531	194	0
1	E	3626	0	3531	187	0
1	F	3626	0	3531	193	0
1	G	3626	0	3531	190	0
1	H	3626	0	3531	192	0
1	I	3626	0	3531	189	0
1	J	3626	0	3531	192	0
1	K	3626	0	3531	188	0
1	L	3626	0	3531	193	0
2	M	2861	0	2826	144	0
2	N	2861	0	2826	152	0
2	O	2861	0	2826	149	0
2	P	2861	0	2826	155	0
2	Q	2861	0	2826	149	0
2	R	2861	0	2826	147	0
2	S	2861	0	2826	152	0
2	T	2861	0	2826	146	0
2	U	2861	0	2826	153	0
2	V	2861	0	2826	151	0
2	W	2861	0	2826	152	0
2	X	2861	0	2826	144	0
3	M	23	0	21	0	0
3	N	23	0	21	0	0
3	O	23	0	21	0	0
3	P	23	0	21	0	0
3	Q	23	0	21	0	0
3	R	23	0	21	0	0
3	S	23	0	21	0	0
3	T	23	0	21	0	0
3	U	23	0	21	0	0
3	V	23	0	21	0	0
3	W	23	0	21	0	0
3	X	23	0	21	0	0
All	All	78120	0	76536	3377	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 22.

The worst 5 of 3377 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:K:43:PHE:HB3	2:W:370:LYS:CE	1.36	1.55
1:B:43:PHE:HB3	2:N:370:LYS:CE	1.36	1.55
1:L:43:PHE:HB3	2:X:370:LYS:CE	1.36	1.54
1:A:43:PHE:HB3	2:M:370:LYS:CE	1.36	1.54
1:E:43:PHE:HB3	2:Q:370:LYS:CE	1.36	1.51

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	B	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	C	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	D	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	E	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	F	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	G	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	11	55
1	H	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	I	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	J	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	K	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	11	55
1	L	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	N	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	O	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	P	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	Q	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	R	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	S	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	T	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	U	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	V	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	W	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
2	X	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	24	69
All	All	9984/10032 (100%)	9278 (93%)	574 (6%)	132 (1%)	20	59

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO

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 PDB entries followed by that with respect to all EM entries.

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	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	B	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	C	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	D	383/383 (100%)	348 (91%)	35 (9%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	383/383 (100%)	347 (91%)	36 (9%)	11	42
1	F	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	G	383/383 (100%)	347 (91%)	36 (9%)	11	42
1	H	383/383 (100%)	347 (91%)	36 (9%)	11	42
1	I	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	J	383/383 (100%)	347 (91%)	36 (9%)	11	42
1	K	383/383 (100%)	348 (91%)	35 (9%)	12	43
1	L	383/383 (100%)	348 (91%)	35 (9%)	12	43
2	M	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	N	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	O	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	P	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	Q	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	R	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	S	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	T	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	U	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	V	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	W	292/297 (98%)	256 (88%)	36 (12%)	6	30
2	X	292/297 (98%)	256 (88%)	36 (12%)	6	30
All	All	8100/8160 (99%)	7244 (89%)	856 (11%)	13	36

5 of 856 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	464	LEU
2	N	160	LEU
2	W	46	LYS
1	L	96	THR
2	M	87	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	277	ASN
1	J	244	ASN
2	U	218	ASN
1	H	384	ASN
1	I	264	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	MAL	M	401	-	24,24,24	1.12	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	N	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	O	401	-	24,24,24	1.12	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	P	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	Q	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	R	401	-	24,24,24	1.12	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	S	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	6 (17%)
3	MAL	T	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAL	U	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	V	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	W	401	-	24,24,24	1.11	1 (4%)	35,35,35	1.79	7 (20%)
3	MAL	X	401	-	24,24,24	1.12	1 (4%)	35,35,35	1.79	7 (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	MAL	M	401	-	-	0/8/48/48	0/2/2/2
3	MAL	N	401	-	-	0/8/48/48	0/2/2/2
3	MAL	O	401	-	-	0/8/48/48	0/2/2/2
3	MAL	P	401	-	-	0/8/48/48	0/2/2/2
3	MAL	Q	401	-	-	0/8/48/48	0/2/2/2
3	MAL	R	401	-	-	0/8/48/48	0/2/2/2
3	MAL	S	401	-	-	0/8/48/48	0/2/2/2
3	MAL	T	401	-	-	0/8/48/48	0/2/2/2
3	MAL	U	401	-	-	0/8/48/48	0/2/2/2
3	MAL	V	401	-	-	0/8/48/48	0/2/2/2
3	MAL	W	401	-	-	0/8/48/48	0/2/2/2
3	MAL	X	401	-	-	0/8/48/48	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	401	MAL	O5'-C1'	-3.01	1.37	1.43
3	O	401	MAL	O5'-C1'	-2.98	1.37	1.43
3	N	401	MAL	O5'-C1'	-2.98	1.37	1.43
3	X	401	MAL	O5'-C1'	-2.97	1.37	1.43
3	Q	401	MAL	O5'-C1'	-2.96	1.37	1.43

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	401	MAL	O1'-C1'-O5'	-4.19	98.64	110.33
3	S	401	MAL	O1'-C1'-O5'	-4.18	98.67	110.33
3	W	401	MAL	O1'-C1'-O5'	-4.18	98.68	110.33
3	U	401	MAL	O1'-C1'-O5'	-4.17	98.70	110.33
3	T	401	MAL	O1'-C1'-O5'	-4.17	98.70	110.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
2	P	1
2	Q	1
2	V	1
2	W	1
2	T	1
2	N	1
2	U	1
2	X	1
2	O	1
2	R	1
2	S	1
2	M	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	369:THR	C	370:LYS	N	1.68
1	O	369:THR	C	370:LYS	N	1.68
1	P	369:THR	C	370:LYS	N	1.68
1	Q	369:THR	C	370:LYS	N	1.68
1	T	369:THR	C	370:LYS	N	1.68