



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 10:52 AM EDT

PDB ID : 4TQV / pdb_00004tqv
Title : Crystal structure of a bacterial ABC transporter involved in the import of the acidic polysaccharide alginate
Authors : Maruyama, Y.; Itoh, T.; Kaneko, A.; Nishitani, Y.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on : 2014-06-12
Resolution : 4.50 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
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

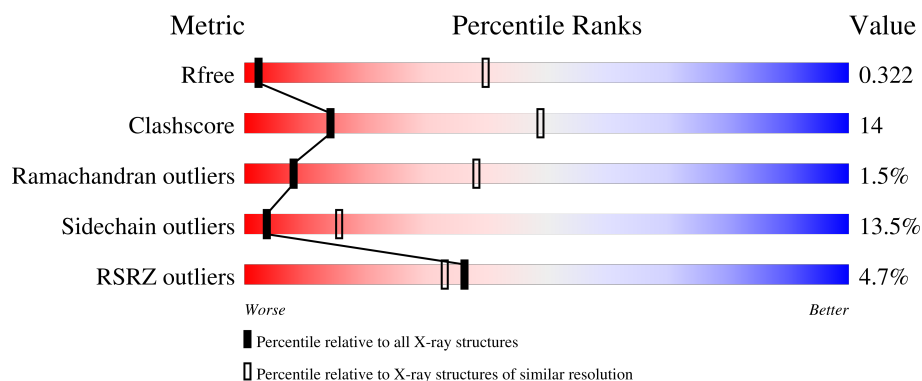
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	301	
1	E	301	
1	I	301	
1	M	301	
2	B	305	

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Mol	Chain	Length	Quality of chain
2	F	305	
2	J	305	
2	N	305	
3	C	363	
3	D	363	
3	G	363	
3	H	363	
3	K	363	
3	L	363	
3	O	363	
3	P	363	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 40472 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 AlgM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	E	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	I	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	M	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q9KWT8
E	24	MET	-	expression tag	UNP Q9KWT8
I	24	MET	-	expression tag	UNP Q9KWT8
M	24	MET	-	expression tag	UNP Q9KWT8

- Molecule 2 is a protein called AlgM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			
2	F	280	Total	C	N	O	S	0	0	0
			2229	1488	354	375	12			
2	J	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			
2	N	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	LEU	-	expression tag	UNP Q9KWT7
B	295	GLU	-	expression tag	UNP Q9KWT7
B	296	HIS	-	expression tag	UNP Q9KWT7
B	297	HIS	-	expression tag	UNP Q9KWT7
B	298	HIS	-	expression tag	UNP Q9KWT7
B	299	HIS	-	expression tag	UNP Q9KWT7
B	300	HIS	-	expression tag	UNP Q9KWT7
B	301	HIS	-	expression tag	UNP Q9KWT7
B	302	HIS	-	expression tag	UNP Q9KWT7
B	303	HIS	-	expression tag	UNP Q9KWT7
B	304	HIS	-	expression tag	UNP Q9KWT7
B	305	HIS	-	expression tag	UNP Q9KWT7
F	294	LEU	-	expression tag	UNP Q9KWT7
F	295	GLU	-	expression tag	UNP Q9KWT7
F	296	HIS	-	expression tag	UNP Q9KWT7
F	297	HIS	-	expression tag	UNP Q9KWT7
F	298	HIS	-	expression tag	UNP Q9KWT7
F	299	HIS	-	expression tag	UNP Q9KWT7
F	300	HIS	-	expression tag	UNP Q9KWT7
F	301	HIS	-	expression tag	UNP Q9KWT7
F	302	HIS	-	expression tag	UNP Q9KWT7
F	303	HIS	-	expression tag	UNP Q9KWT7
F	304	HIS	-	expression tag	UNP Q9KWT7
F	305	HIS	-	expression tag	UNP Q9KWT7
J	294	LEU	-	expression tag	UNP Q9KWT7
J	295	GLU	-	expression tag	UNP Q9KWT7
J	296	HIS	-	expression tag	UNP Q9KWT7
J	297	HIS	-	expression tag	UNP Q9KWT7
J	298	HIS	-	expression tag	UNP Q9KWT7
J	299	HIS	-	expression tag	UNP Q9KWT7
J	300	HIS	-	expression tag	UNP Q9KWT7
J	301	HIS	-	expression tag	UNP Q9KWT7
J	302	HIS	-	expression tag	UNP Q9KWT7
J	303	HIS	-	expression tag	UNP Q9KWT7
J	304	HIS	-	expression tag	UNP Q9KWT7
J	305	HIS	-	expression tag	UNP Q9KWT7
N	294	LEU	-	expression tag	UNP Q9KWT7
N	295	GLU	-	expression tag	UNP Q9KWT7
N	296	HIS	-	expression tag	UNP Q9KWT7
N	297	HIS	-	expression tag	UNP Q9KWT7
N	298	HIS	-	expression tag	UNP Q9KWT7
N	299	HIS	-	expression tag	UNP Q9KWT7
N	300	HIS	-	expression tag	UNP Q9KWT7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	301	HIS	-	expression tag	UNP Q9KWT7
N	302	HIS	-	expression tag	UNP Q9KWT7
N	303	HIS	-	expression tag	UNP Q9KWT7
N	304	HIS	-	expression tag	UNP Q9KWT7
N	305	HIS	-	expression tag	UNP Q9KWT7

- Molecule 3 is a protein called AlgS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	D	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	G	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	H	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	K	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	L	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	O	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	P	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			

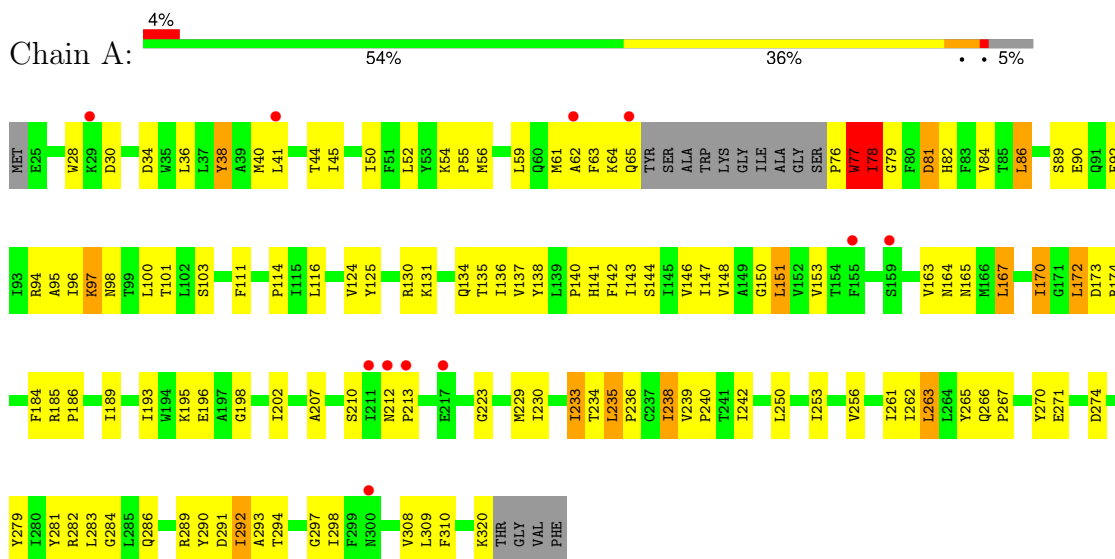
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	GLU	engineered mutation	UNP Q9KWT9
D	160	GLN	GLU	engineered mutation	UNP Q9KWT9
G	160	GLN	GLU	engineered mutation	UNP Q9KWT9
H	160	GLN	GLU	engineered mutation	UNP Q9KWT9
K	160	GLN	GLU	engineered mutation	UNP Q9KWT9
L	160	GLN	GLU	engineered mutation	UNP Q9KWT9
O	160	GLN	GLU	engineered mutation	UNP Q9KWT9
P	160	GLN	GLU	engineered mutation	UNP Q9KWT9

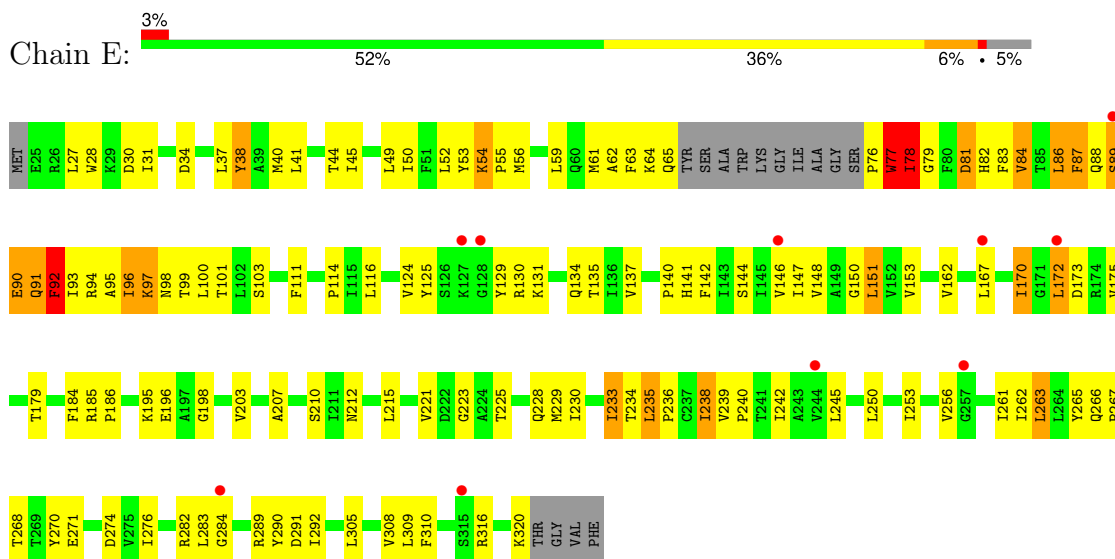
3 Residue-property plots [i](#)

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.

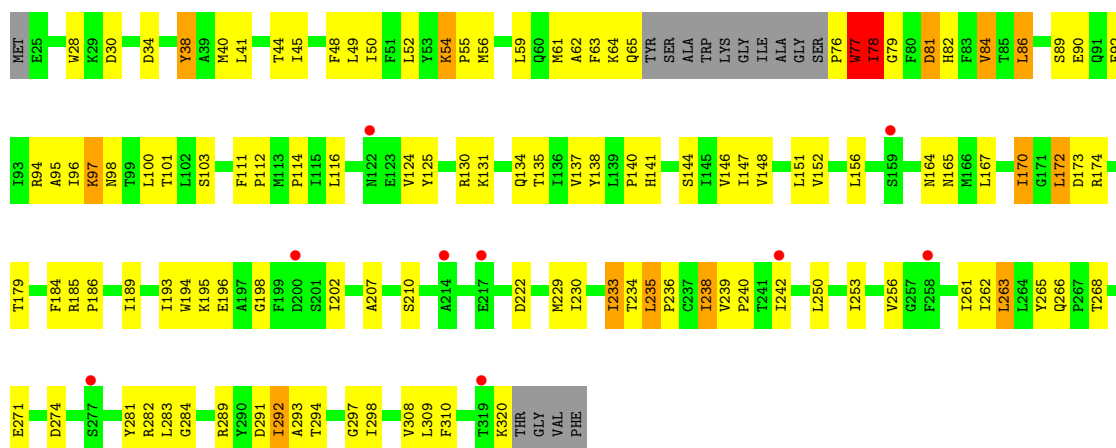
- Molecule 1: AlgM1



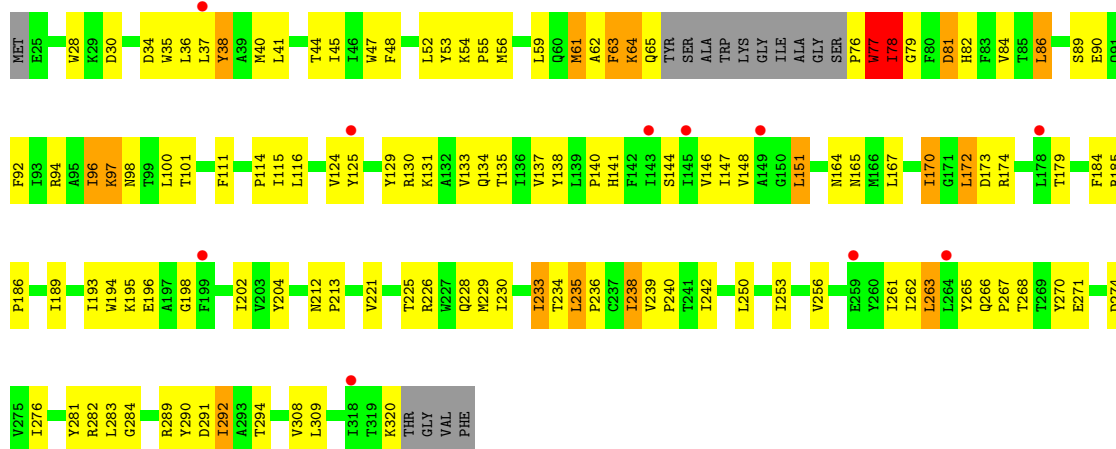
- Molecule 1: AlgM1



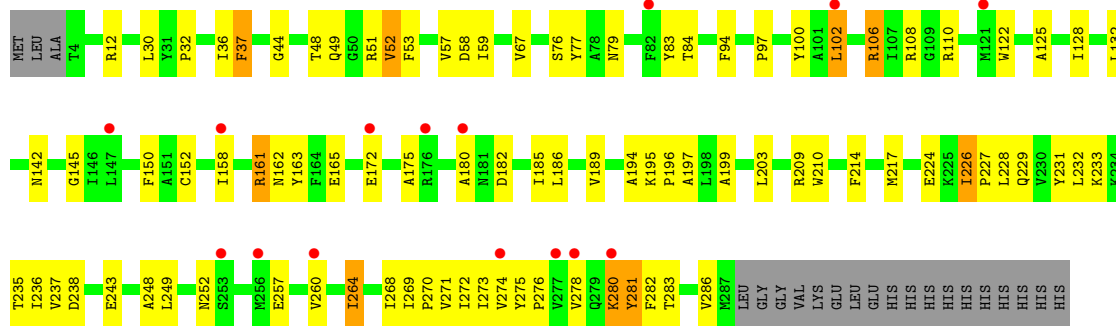
- Molecule 1: AlgM1



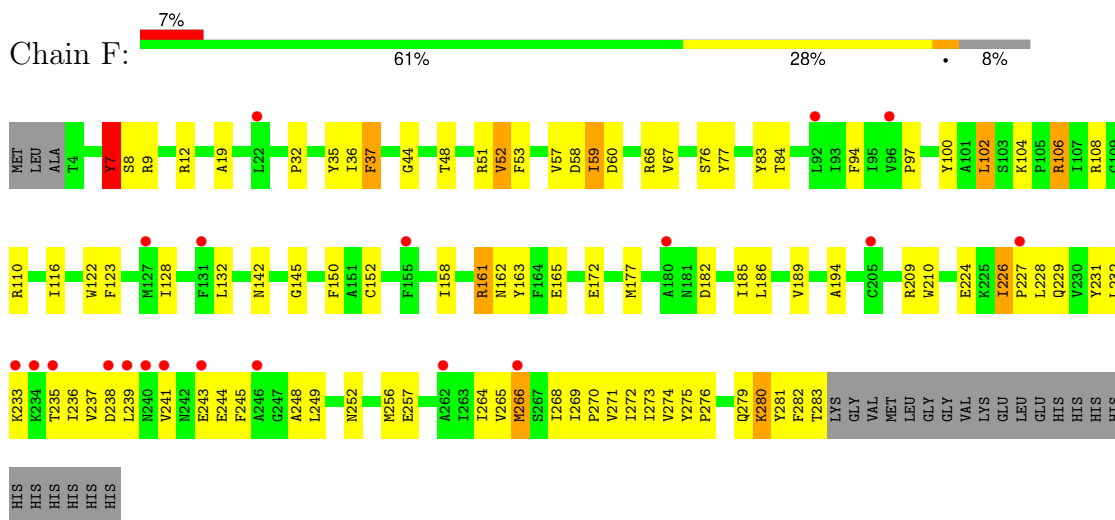
• Molecule 1: AlgM1



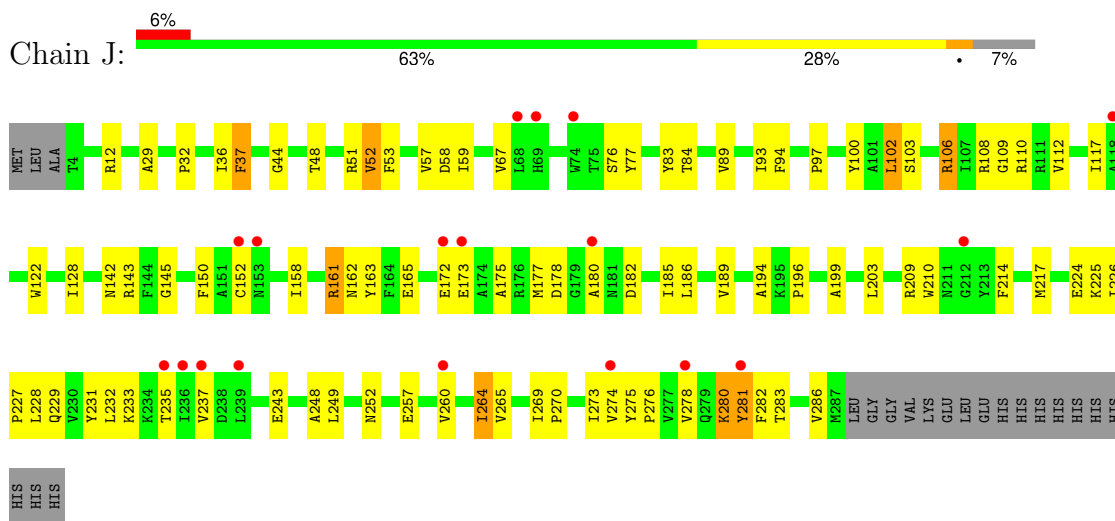
• Molecule 2: AlgM2



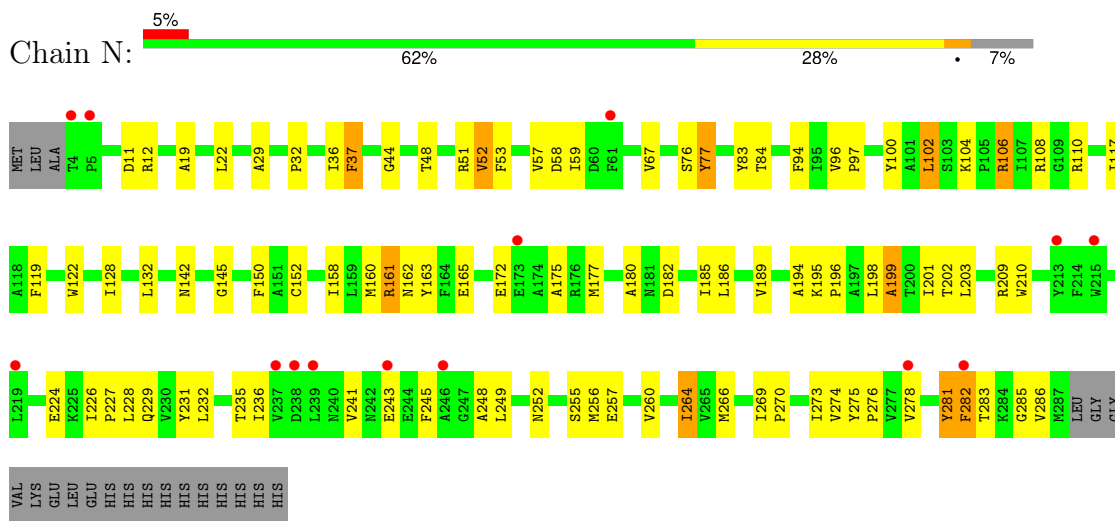
• Molecule 2: AlgM2



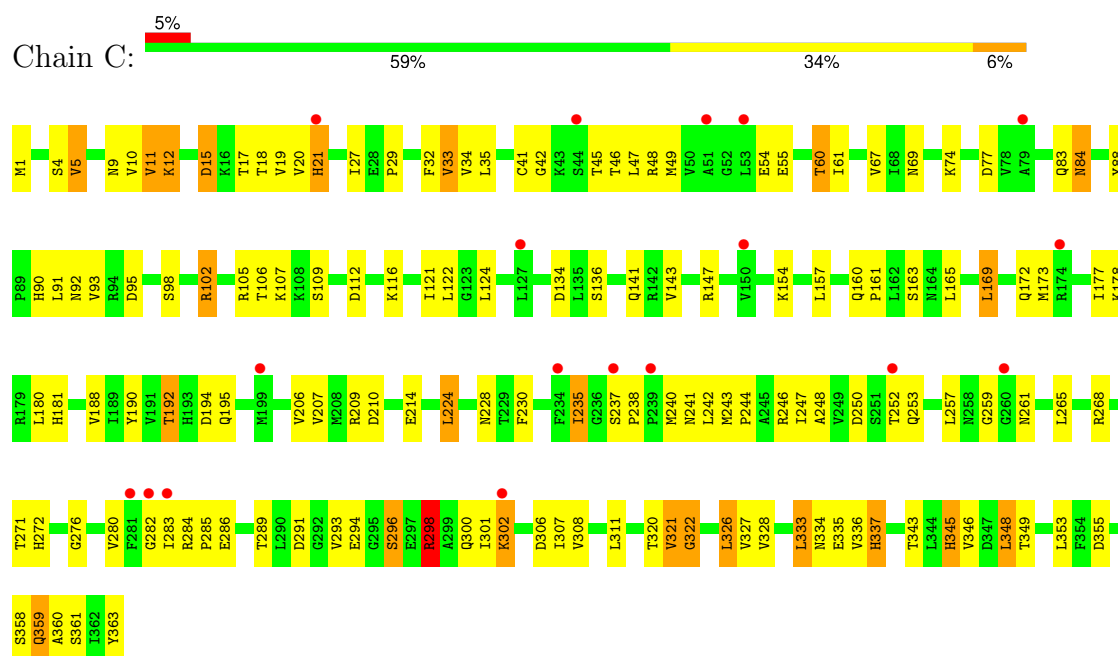
• Molecule 2: AlgM2



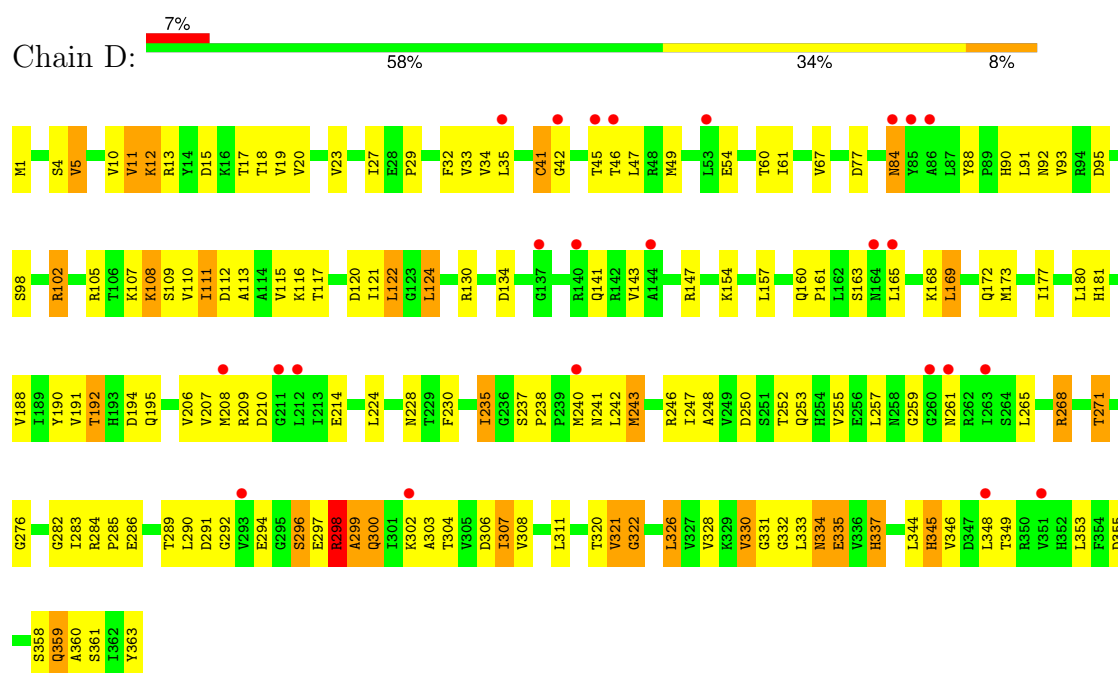
• Molecule 2: AlgM2



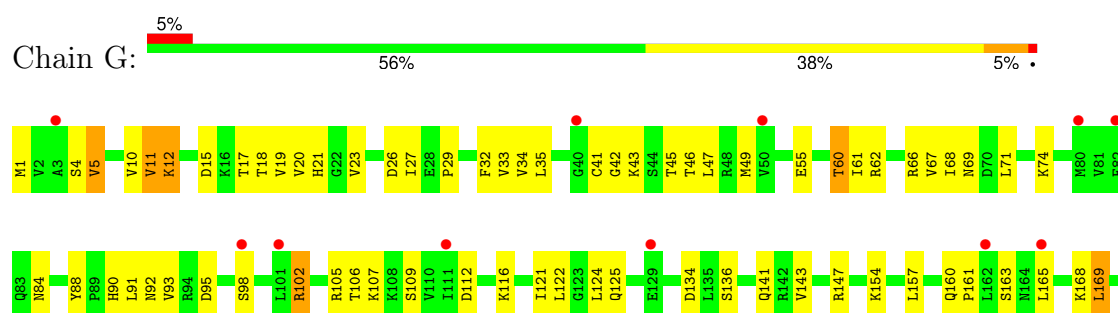
• Molecule 3: AlgS

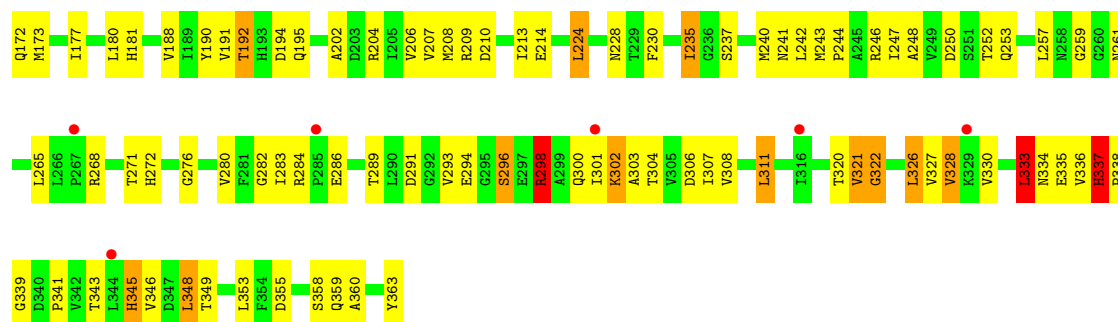


• Molecule 3: AlgS

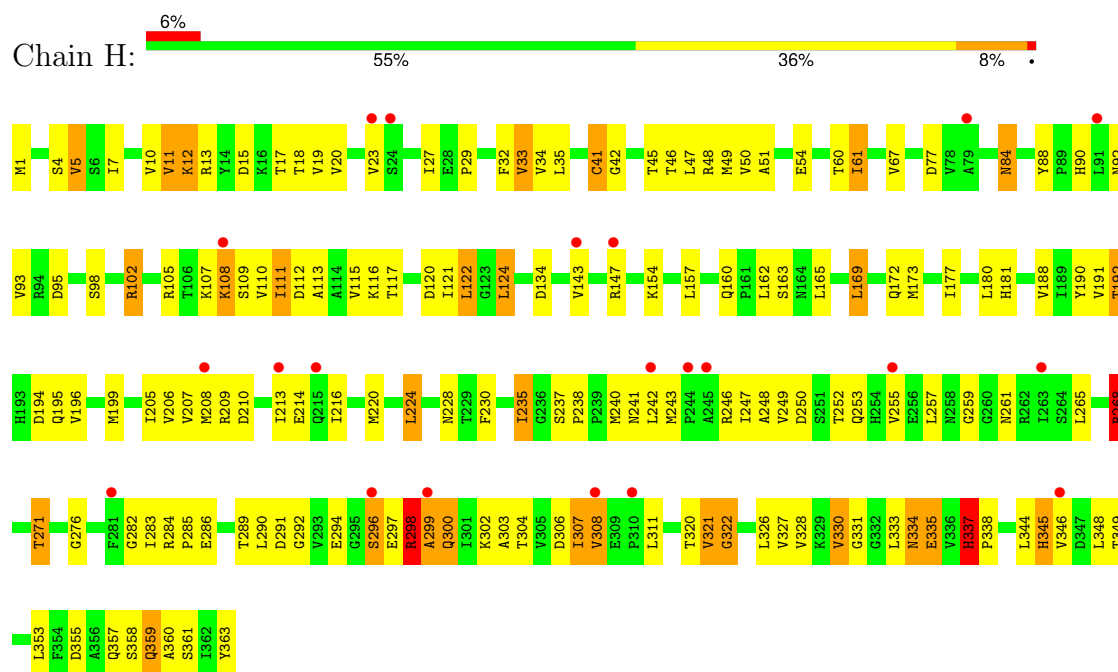


• Molecule 3: AlgS





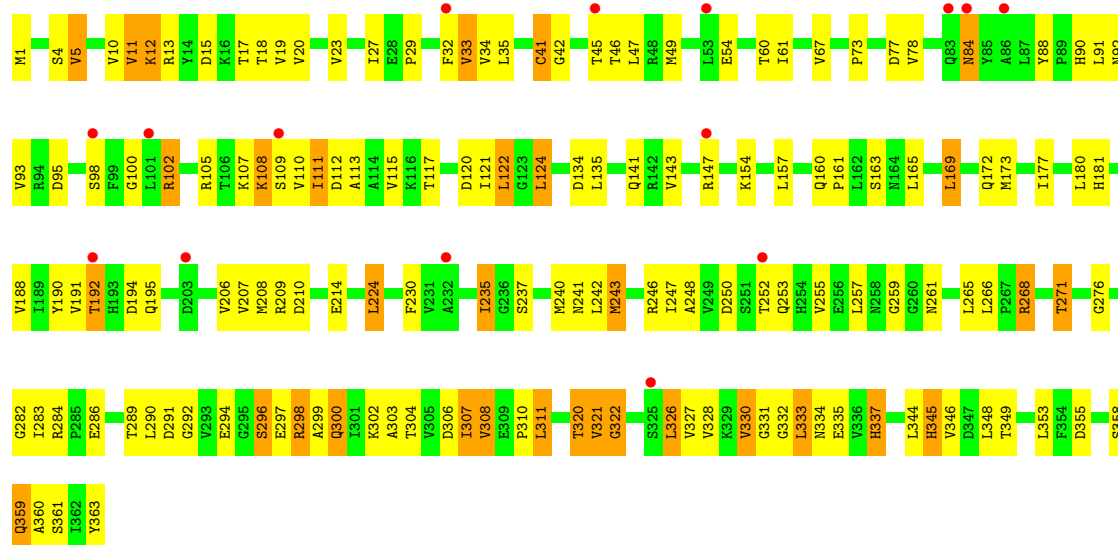
- Molecule 3: AlgS



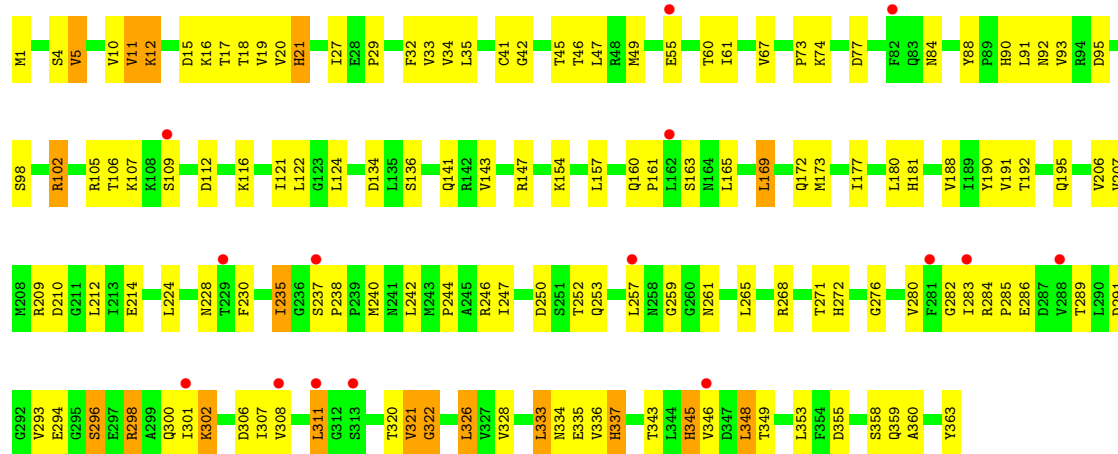
- Molecule 3: AlgS



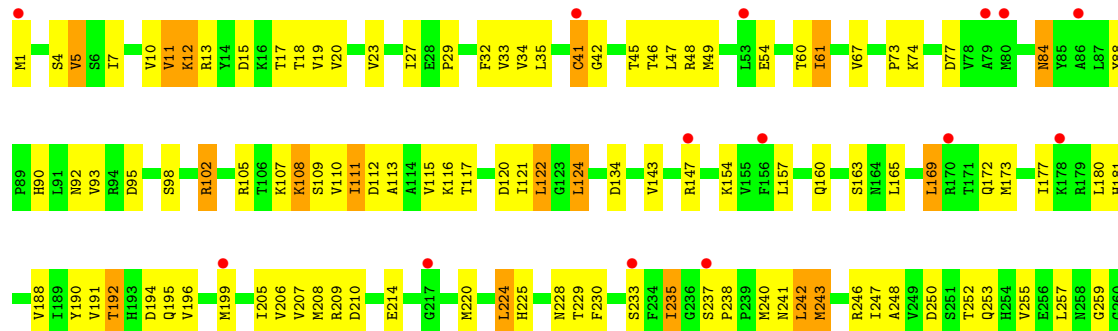
- Molecule 3: AlgS

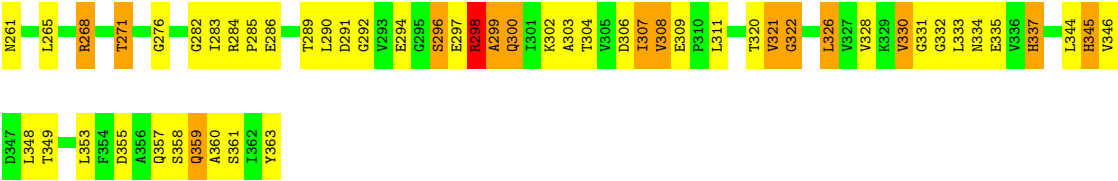


• Molecule 3: Algs



• Molecule 3: Algs





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.25Å 151.19Å 162.41Å 68.66° 81.76° 90.10°	Depositor
Resolution (Å)	29.82 – 4.50 29.82 – 4.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.82-4.50) 80.1 (29.82-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.279 , 0.320 0.282 , 0.322	Depositor DCC
R_{free} test set	2000 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	169.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	40472	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

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	0.35	0/2377	0.80	1/3241 (0.0%)
1	E	0.37	0/2377	0.88	6/3241 (0.2%)
1	I	0.34	0/2377	0.80	1/3241 (0.0%)
1	M	0.35	0/2377	0.83	3/3241 (0.1%)
2	B	0.38	0/2316	0.91	5/3149 (0.2%)
2	F	0.38	0/2288	0.93	6/3113 (0.2%)
2	J	0.37	0/2316	0.91	5/3149 (0.2%)
2	N	0.40	1/2316 (0.0%)	0.93	8/3149 (0.3%)
3	C	0.36	0/2822	0.96	7/3826 (0.2%)
3	D	0.38	0/2822	1.00	15/3826 (0.4%)
3	G	0.38	0/2822	1.00	13/3826 (0.3%)
3	H	0.36	0/2822	1.00	14/3826 (0.4%)
3	K	0.37	0/2822	0.95	8/3826 (0.2%)
3	L	0.36	0/2822	1.00	17/3826 (0.4%)
3	O	0.37	0/2822	0.95	5/3826 (0.1%)
3	P	0.36	0/2822	1.00	16/3826 (0.4%)
All	All	0.37	1/41320 (0.0%)	0.94	130/56132 (0.2%)

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	E	0	1
1	I	0	1
1	M	0	1
3	C	0	1
3	K	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	199	ALA	CA-CB	-5.14	1.45	1.53

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	282	PHE	N-CA-C	9.84	123.23	111.82
2	B	282	PHE	N-CA-C	9.44	122.77	111.82
2	N	282	PHE	N-CA-C	9.22	122.51	111.82
2	F	281	TYR	N-CA-C	8.16	120.98	111.02
1	E	91	GLN	CA-C-N	8.06	131.40	120.44

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	TRP	Peptide
3	C	21	HIS	Mainchain
1	E	77	TRP	Peptide
1	I	77	TRP	Peptide
3	K	21	HIS	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2314	0	2402	83	1
1	E	2314	0	2402	90	0
1	I	2314	0	2402	74	1
1	M	2314	0	2402	83	0
2	B	2257	0	2320	64	0
2	F	2229	0	2286	64	1
2	J	2257	0	2320	65	0
2	N	2257	0	2320	72	1
3	C	2777	0	2854	78	0
3	D	2777	0	2854	80	0
3	G	2777	0	2854	92	0
3	H	2777	0	2854	91	0
3	K	2777	0	2854	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2777	0	2854	87	0
3	O	2777	0	2854	74	0
3	P	2777	0	2854	89	0
All	All	40472	0	41686	1170	2

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 14.

The worst 5 of 1170 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:M:34:ASP:OD1	2:N:106:ARG:NH1	1.72	1.23
1:E:34:ASP:OD1	2:F:106:ARG:NH1	2.02	0.92
2:N:102:LEU:HD12	2:N:161:ARG:HE	1.40	0.87
3:L:195:GLN:HG3	3:L:235:ILE:HA	1.59	0.84
2:N:76:SER:HB3	2:N:228:LEU:H	1.42	0.84

All (2) 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:I:289:ARG:NH1	2:N:241:VAL:O[1_654]	2.08	0.12
1:A:289:ARG:NH1	2:F:241:VAL:O[1_654]	2.09	0.11

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	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	30	67
1	E	282/301 (94%)	252 (89%)	26 (9%)	4 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	30	67
1	M	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	30	67
2	B	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
2	F	278/305 (91%)	243 (87%)	32 (12%)	3 (1%)	11	45
2	J	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
2	N	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
3	C	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	D	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	G	361/363 (99%)	321 (89%)	35 (10%)	5 (1%)	9	39
3	H	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	K	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	L	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	O	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	P	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
All	All	5140/5328 (96%)	4583 (89%)	478 (9%)	79 (2%)	8	38

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ILE
3	C	18	THR
3	C	322	GLY
3	C	336	VAL
3	C	359	GLN

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	250/260 (96%)	217 (87%)	33 (13%)	4	16
1	E	250/260 (96%)	216 (86%)	34 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	250/260 (96%)	217 (87%)	33 (13%)	4	16
1	M	250/260 (96%)	218 (87%)	32 (13%)	4	17
2	B	240/258 (93%)	223 (93%)	17 (7%)	13	35
2	F	237/258 (92%)	218 (92%)	19 (8%)	11	32
2	J	240/258 (93%)	223 (93%)	17 (7%)	13	35
2	N	240/258 (93%)	224 (93%)	16 (7%)	15	37
3	C	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	D	307/307 (100%)	254 (83%)	53 (17%)	2	11
3	G	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	H	307/307 (100%)	254 (83%)	53 (17%)	2	11
3	K	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	L	307/307 (100%)	255 (83%)	52 (17%)	2	11
3	O	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	P	307/307 (100%)	253 (82%)	54 (18%)	2	11
All	All	4413/4528 (98%)	3816 (86%)	597 (14%)	4	16

5 of 597 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	97	LYS
3	P	252	THR
1	M	265	TYR
1	M	96	ILE
3	O	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	21	HIS
1	M	220	GLN
3	L	90	HIS
3	L	357	GLN
2	N	279	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	286/301 (95%)	0.00	11 (3%)	44	37	45, 123, 232, 396	0
1	E	286/301 (95%)	-0.04	10 (3%)	47	38	72, 144, 245, 389	0
1	I	286/301 (95%)	0.07	9 (3%)	51	40	63, 110, 236, 381	0
1	M	286/301 (95%)	0.01	10 (3%)	47	38	63, 137, 231, 308	0
2	B	284/305 (93%)	0.11	15 (5%)	32	30	40, 135, 260, 432	0
2	F	280/305 (91%)	0.21	20 (7%)	22	24	74, 138, 252, 482	0
2	J	284/305 (93%)	0.11	18 (6%)	26	27	64, 129, 253, 401	0
2	N	284/305 (93%)	0.08	14 (4%)	35	32	50, 112, 244, 387	0
3	C	363/363 (100%)	0.17	18 (4%)	34	31	44, 179, 275, 344	0
3	D	363/363 (100%)	0.27	24 (6%)	24	26	72, 187, 302, 373	0
3	G	363/363 (100%)	0.21	17 (4%)	36	33	70, 160, 285, 349	0
3	H	363/363 (100%)	0.21	21 (5%)	29	29	46, 146, 267, 367	0
3	K	363/363 (100%)	0.09	10 (2%)	55	43	47, 156, 263, 338	0
3	L	363/363 (100%)	0.08	15 (4%)	41	36	69, 154, 276, 340	0
3	O	363/363 (100%)	0.23	15 (4%)	41	36	65, 198, 291, 376	0
3	P	363/363 (100%)	0.13	14 (3%)	43	37	57, 162, 279, 355	0
All	All	5180/5328 (97%)	0.13	241 (4%)	36	33	40, 151, 275, 482	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	4	THR	8.0
2	B	278	VAL	7.2
3	O	237	SER	7.0
2	J	239	LEU	7.0
3	K	86	ALA	6.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.