wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4TQV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

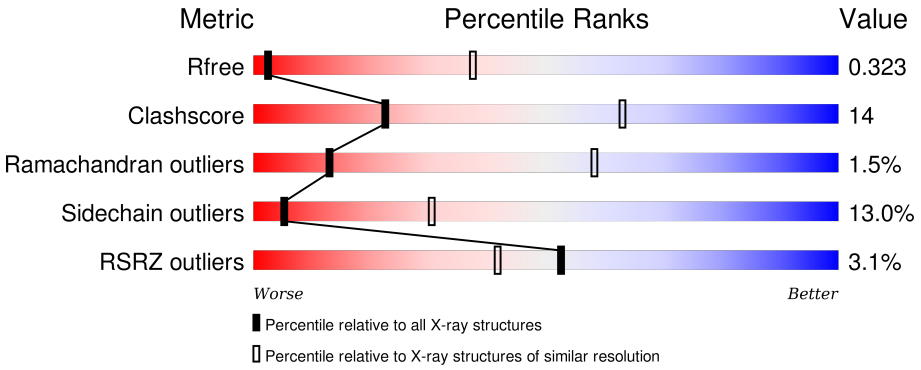
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	54% 37% • • 5%
1	E	301	2% 53% 36% 5% • 5%
1	I	301	56% 34% • • 5%
1	M	301	% 55% 35% • • 5%
2	B	305	2% 64% 26% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	305	2% 62% 26% 8%
2	J	305	2% 64% 26% 7%
2	N	305	2% 63% 27% 7%
3	C	363	3% 61% 33% 6%
3	D	363	7% 62% 31% 7%
3	G	363	3% 59% 35% 6%
3	H	363	4% 58% 34% 7%
3	K	363	2% 64% 31% 6%
3	L	363	5% 62% 31% 8%
3	O	363	7% 63% 32% 5%
3	P	363	4% 60% 33% 7%

2 Entry composition

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

Continued on next page...

Continued from previous page...

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:

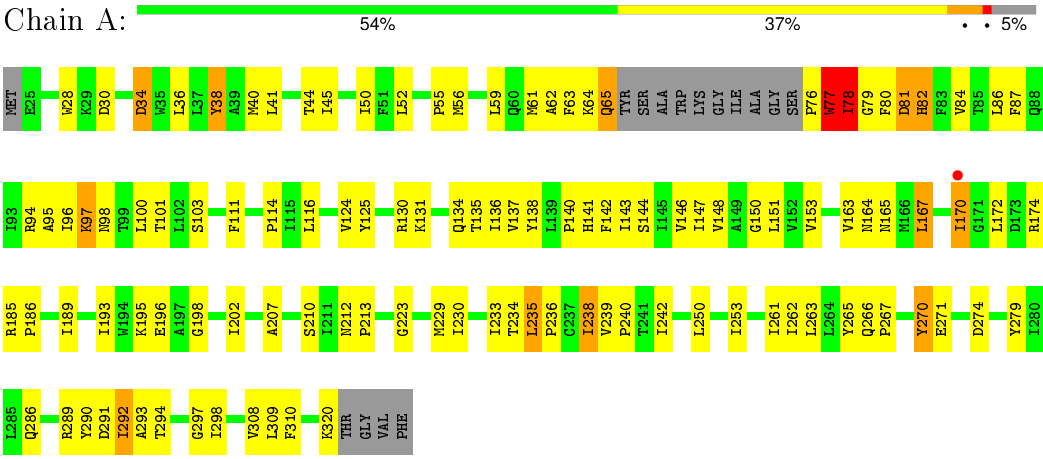
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	GLU	engineered mutation	UNP Q9KWT9
D	160	GLN	GLU	engineered mutation	UNP Q9KWT9
G	160	GLN	GLU	engineered mutation	UNP Q9KWT9
H	160	GLN	GLU	engineered mutation	UNP Q9KWT9
K	160	GLN	GLU	engineered mutation	UNP Q9KWT9
L	160	GLN	GLU	engineered mutation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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

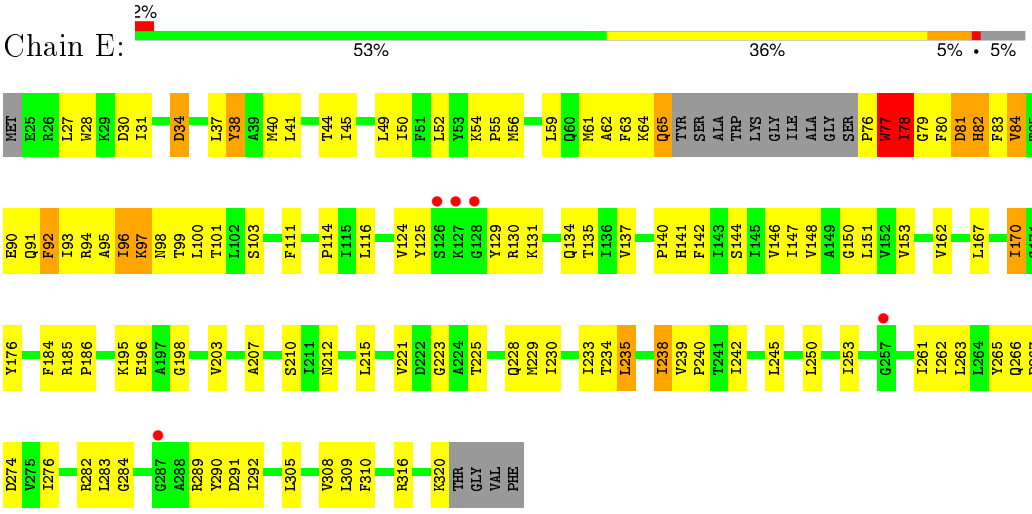
- Molecule 1: AlgM1

Chain A:



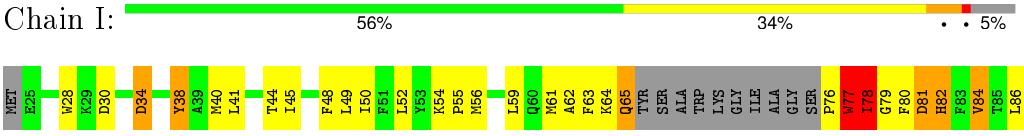
- Molecule 1: AlgM1

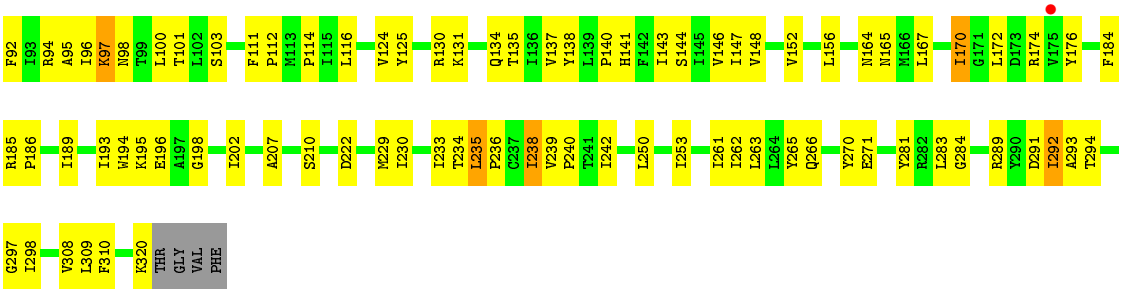
Chain E:



- Molecule 1: AlgM1

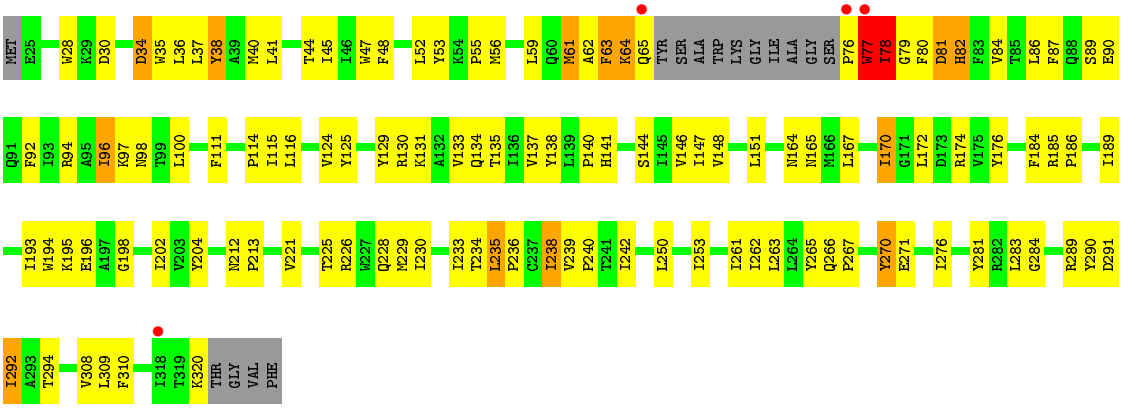
Chain I:





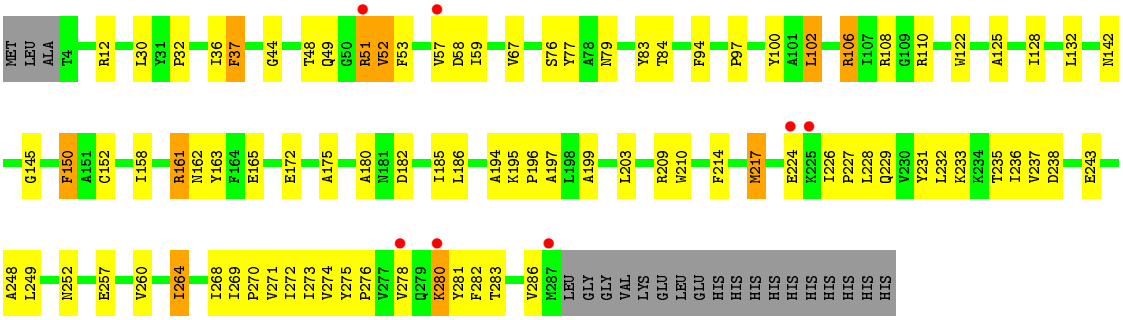
• Molecule 1: AlgM1

Chain M:



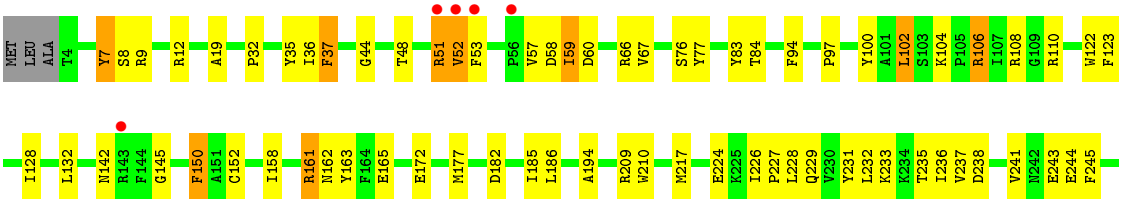
• Molecule 2: AlgM2

Chain B:



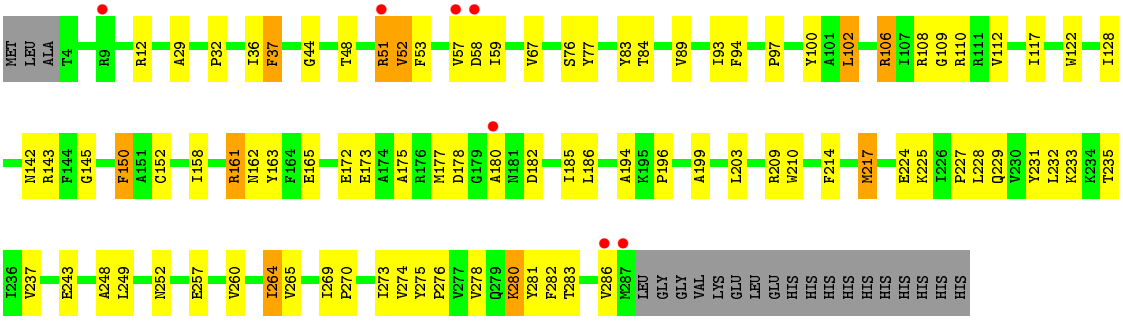
• Molecule 2: AlgM2

Chain F:



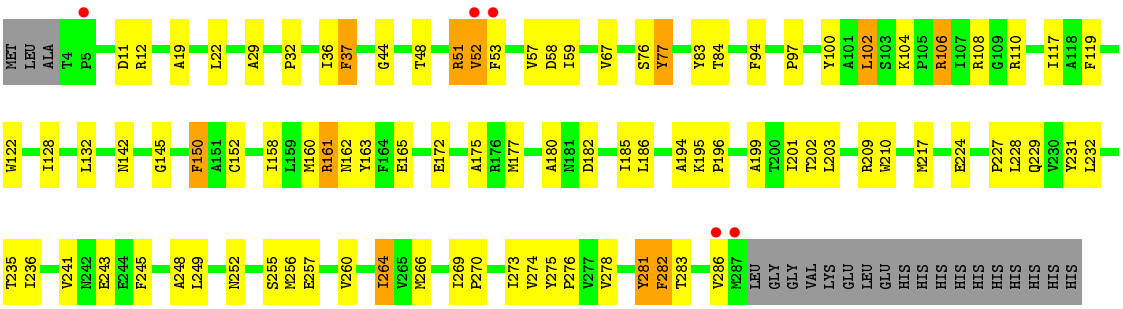
• Molecule 2: AlgM2

Chain J:



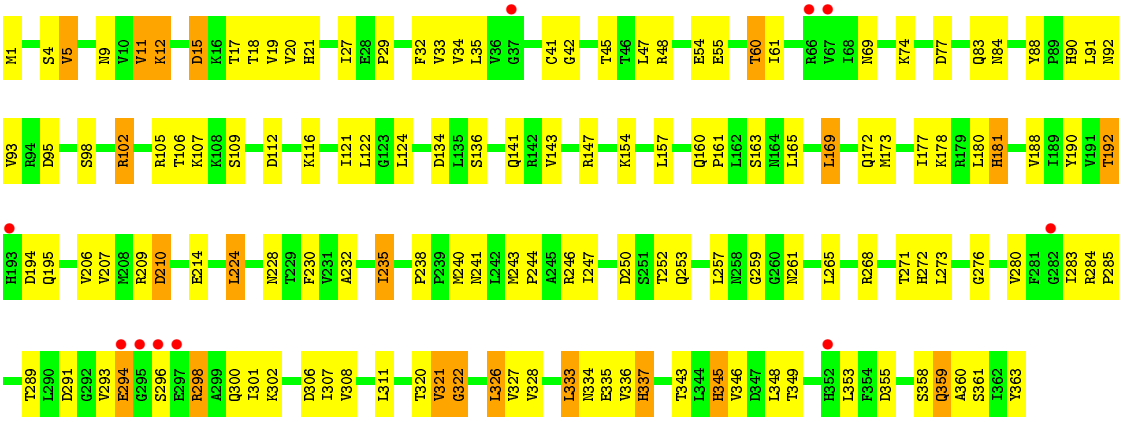
• Molecule 2: AlgM2

Chain N:



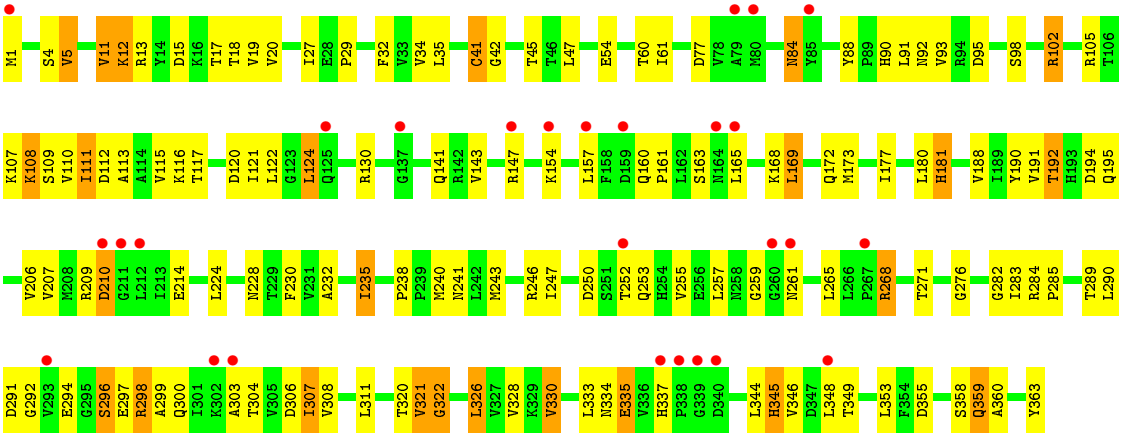
• Molecule 3: AlgS

Chain C:



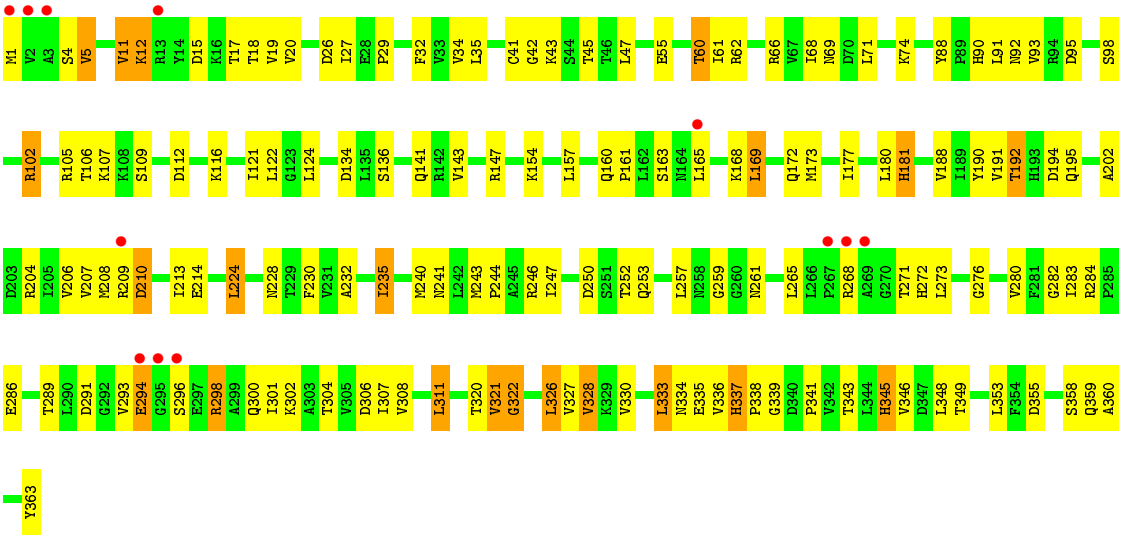
• Molecule 3: AlgS

Chain D:



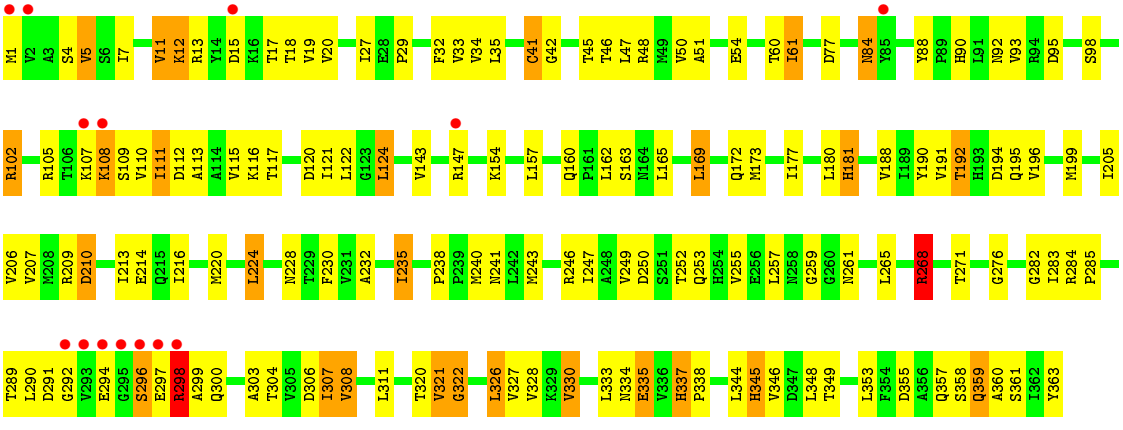
• Molecule 3: AlgS

Chain G:



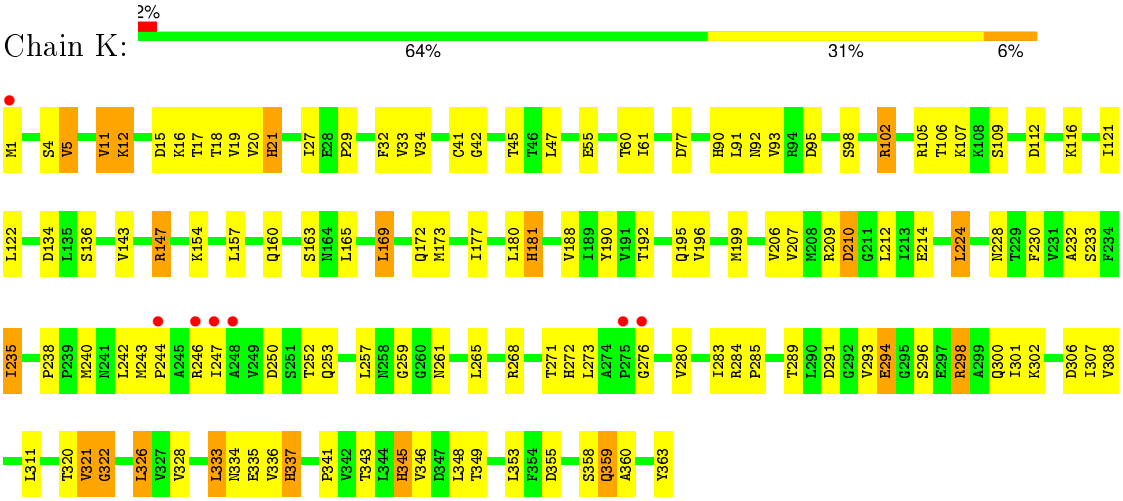
• Molecule 3: AlgS

Chain H:



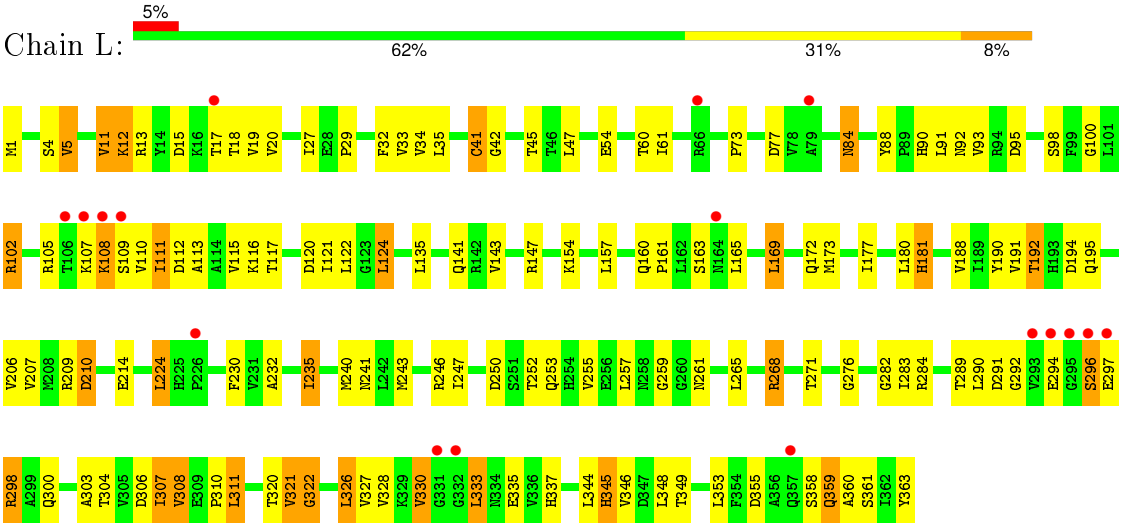
- Molecule 3: AlgS

Chain K:



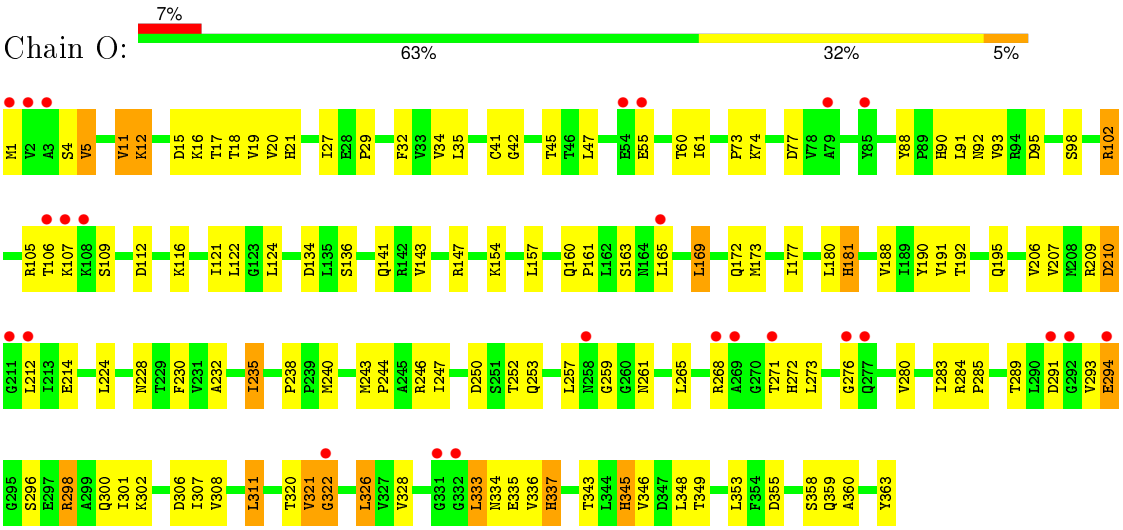
- Molecule 3: AlgS

Chain L:



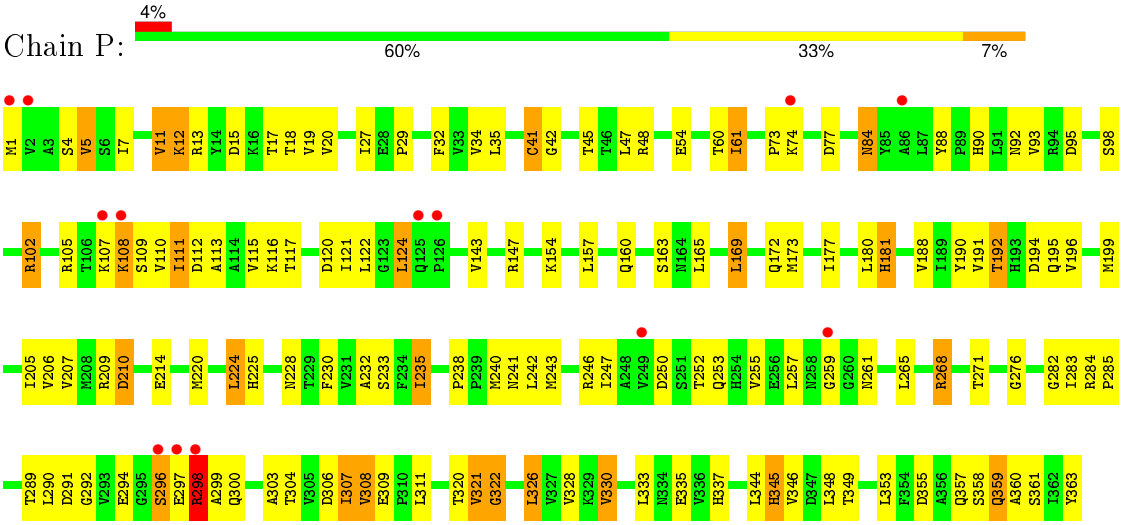
- Molecule 3: AlgS

Chain O:



• Molecule 3: AlgS

Chain P:



4 Data and refinement statistics (i)

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) 71.7 (29.82-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.279 , 0.320 0.277 , 0.323	Depositor DCC
R_{free} test set	1688 reflections (3.54%)	DCC
Wilson B-factor (Å^2)	175.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 57112 reflections	Xtriage
F_o,F_c correlation	0.88	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 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	0/2377	0.48	1/3241 (0.0%)
1	E	0.25	0/2377	0.52	1/3241 (0.0%)
1	I	0.24	0/2377	0.47	1/3241 (0.0%)
1	M	0.24	0/2377	0.49	2/3241 (0.1%)
2	B	0.26	0/2316	0.50	1/3149 (0.0%)
2	F	0.26	0/2288	0.52	1/3113 (0.0%)
2	J	0.26	0/2316	0.50	1/3149 (0.0%)
2	N	0.28	0/2316	0.53	2/3149 (0.1%)
3	C	0.25	0/2822	0.56	0/3826
3	D	0.26	0/2822	0.60	0/3826
3	G	0.26	0/2822	0.59	0/3826
3	H	0.25	0/2822	0.61	2/3826 (0.1%)
3	K	0.26	0/2822	0.57	0/3826
3	L	0.25	0/2822	0.60	0/3826
3	O	0.26	0/2822	0.56	0/3826
3	P	0.26	0/2822	0.62	2/3826 (0.1%)
All	All	0.26	0/41320	0.55	14/56132 (0.0%)

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

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	298	ARG	NE-CZ-NH1	-7.79	116.41	120.30
2	N	282	PHE	CB-CA-C	-6.60	97.20	110.40
2	J	282	PHE	CB-CA-C	-5.93	98.55	110.40
3	H	298	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	P	298	ARG	CA-CB-CG	5.56	125.64	113.40

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2314	0	2402	81	1
1	E	2314	0	2402	82	0
1	I	2314	0	2402	72	1
1	M	2314	0	2402	79	0
2	B	2257	0	2320	63	0
2	F	2229	0	2286	60	1
2	J	2257	0	2320	62	0
2	N	2257	0	2320	71	1
3	C	2777	0	2854	76	0
3	D	2777	0	2854	77	0
3	G	2777	0	2854	90	0
3	H	2777	0	2854	90	0
3	K	2777	0	2854	71	0
3	L	2777	0	2854	84	0
3	O	2777	0	2854	70	0
3	P	2777	0	2854	86	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	40472	0	41686	1126	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 1126 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
2:N:76:SER:HB3	2:N:228:LEU:H	1.42	0.84
3:L:195:GLN:HG3	3:L:235:ILE:HA	1.59	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%)	39 80
1	E	282/301 (94%)	252 (89%)	26 (9%)	4 (1%)	14 59
1	I	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	39 80
1	M	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	39 80
2	B	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	26 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	278/305 (91%)	243 (87%)	32 (12%)	3 (1%)	17 64
2	J	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	26 71
2	N	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	26 71
3	C	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	11 56
3	D	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	6 46
3	G	361/363 (99%)	321 (89%)	35 (10%)	5 (1%)	14 59
3	H	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	6 46
3	K	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	11 56
3	L	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	6 46
3	O	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	11 56
3	P	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	6 46
All	All	5140/5328 (96%)	4583 (89%)	478 (9%)	79 (2%)	13 58

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 (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	250/260 (96%)	218 (87%)	32 (13%)	5 31
1	E	250/260 (96%)	217 (87%)	33 (13%)	5 30
1	I	250/260 (96%)	218 (87%)	32 (13%)	5 31
1	M	250/260 (96%)	219 (88%)	31 (12%)	6 32
2	B	240/258 (93%)	220 (92%)	20 (8%)	14 51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	237/258 (92%)	215 (91%)	22 (9%)	11 45
2	J	240/258 (93%)	220 (92%)	20 (8%)	14 51
2	N	240/258 (93%)	221 (92%)	19 (8%)	15 53
3	C	307/307 (100%)	264 (86%)	43 (14%)	4 28
3	D	307/307 (100%)	259 (84%)	48 (16%)	3 23
3	G	307/307 (100%)	263 (86%)	44 (14%)	4 27
3	H	307/307 (100%)	259 (84%)	48 (16%)	3 23
3	K	307/307 (100%)	264 (86%)	43 (14%)	4 28
3	L	307/307 (100%)	259 (84%)	48 (16%)	3 23
3	O	307/307 (100%)	264 (86%)	43 (14%)	4 28
3	P	307/307 (100%)	259 (84%)	48 (16%)	3 23
All	All	4413/4528 (98%)	3839 (87%)	574 (13%)	5 30

5 of 574 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	181	HIS
1	I	320	LYS
3	P	45	THR
3	H	250	ASP
1	I	30	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	193	HIS
3	K	160	GLN
3	P	160	GLN
3	H	345	HIS
2	J	279	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.40	1 (0%)	94	92	45, 123, 232, 396	0
1	E	286/301 (95%)	-0.38	6 (2%)	67	57	72, 144, 245, 389	0
1	I	286/301 (95%)	-0.36	1 (0%)	94	92	63, 110, 236, 381	0
1	M	286/301 (95%)	-0.34	4 (1%)	78	69	63, 137, 231, 308	0
2	B	284/305 (93%)	-0.27	7 (2%)	61	51	40, 135, 260, 432	0
2	F	280/305 (91%)	-0.34	5 (1%)	71	62	74, 138, 252, 482	0
2	J	284/305 (93%)	-0.35	7 (2%)	61	51	64, 129, 253, 401	0
2	N	284/305 (93%)	-0.42	5 (1%)	71	62	50, 112, 244, 387	0
3	C	363/363 (100%)	-0.13	10 (2%)	56	46	44, 179, 275, 344	0
3	D	363/363 (100%)	0.13	27 (7%)	17	13	72, 187, 302, 373	0
3	G	363/363 (100%)	0.04	12 (3%)	50	40	70, 160, 285, 349	0
3	H	363/363 (100%)	0.00	14 (3%)	43	34	46, 146, 267, 367	0
3	K	363/363 (100%)	-0.18	7 (1%)	70	61	47, 156, 263, 338	0
3	L	363/363 (100%)	-0.04	17 (4%)	35	28	69, 154, 276, 340	0
3	O	363/363 (100%)	0.13	25 (6%)	20	15	65, 198, 291, 376	0
3	P	363/363 (100%)	-0.03	13 (3%)	46	37	57, 162, 279, 355	0
All	All	5180/5328 (97%)	-0.16	161 (3%)	52	42	40, 151, 275, 482	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	1	MET	12.6
3	D	1	MET	8.7
3	O	2	VAL	7.4
3	O	1	MET	7.0
3	D	164	ASN	6.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.