Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Nov 2, 2017 – 07:37 PM EDT

PDB ID	:	5W9N
EMDB ID:	:	EMD-8789
Title	:	MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors	:	Pallesen, J.; Ward, A.B.
Deposited on	:	unknown
Resolution	:	5.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

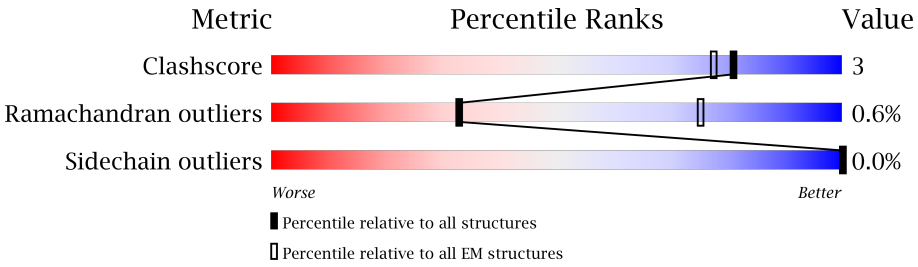
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1329	33% · 65%
1	D	1329	33% · 65%
1	G	1329	33% · 66%
1	H	1329	52% · 45%
1	I	1329	51% · 45%
1	J	1329	52% · 45%
2	B	233	51% 49%
2	E	233	51% 49%
3	C	218	49% · 49%

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Mol	Chain	Length	Quality of chain
3	F	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31126 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 MERS S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	G	457	Total	C	N	O	S	0	0
			3496	2214	590	675	17		
1	H	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	I	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	J	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
D	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
G	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
H	506	PHE	LEU	conflict	UNP W5ZZF5
H	748	ALA	ARG	conflict	UNP W5ZZF5
H	751	GLY	ARG	conflict	UNP W5ZZF5
H	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
H	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
H	1292	GLY	-	expression tag	UNP W5ZZF5
H	1293	SER	-	expression tag	UNP W5ZZF5
H	1294	GLY	-	expression tag	UNP W5ZZF5
H	1295	TYR	-	expression tag	UNP W5ZZF5
H	1296	ILE	-	expression tag	UNP W5ZZF5
H	1297	PRO	-	expression tag	UNP W5ZZF5
H	1298	GLU	-	expression tag	UNP W5ZZF5
H	1299	ALA	-	expression tag	UNP W5ZZF5
H	1300	PRO	-	expression tag	UNP W5ZZF5
H	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1302	ASP	-	expression tag	UNP W5ZZF5
H	1303	GLY	-	expression tag	UNP W5ZZF5
H	1304	GLN	-	expression tag	UNP W5ZZF5
H	1305	ALA	-	expression tag	UNP W5ZZF5
H	1306	TYR	-	expression tag	UNP W5ZZF5
H	1307	VAL	-	expression tag	UNP W5ZZF5
H	1308	ARG	-	expression tag	UNP W5ZZF5
H	1309	LYS	-	expression tag	UNP W5ZZF5
H	1310	ASP	-	expression tag	UNP W5ZZF5
H	1311	GLY	-	expression tag	UNP W5ZZF5
H	1312	GLU	-	expression tag	UNP W5ZZF5
H	1313	TRP	-	expression tag	UNP W5ZZF5
H	1314	VAL	-	expression tag	UNP W5ZZF5
H	1315	LEU	-	expression tag	UNP W5ZZF5
H	1316	LEU	-	expression tag	UNP W5ZZF5
H	1317	SER	-	expression tag	UNP W5ZZF5
H	1318	THR	-	expression tag	UNP W5ZZF5
H	1319	PHE	-	expression tag	UNP W5ZZF5
H	1320	LEU	-	expression tag	UNP W5ZZF5
H	1321	GLY	-	expression tag	UNP W5ZZF5
H	1322	ARG	-	expression tag	UNP W5ZZF5
H	1323	SER	-	expression tag	UNP W5ZZF5
H	1324	LEU	-	expression tag	UNP W5ZZF5
H	1325	GLU	-	expression tag	UNP W5ZZF5
H	1326	VAL	-	expression tag	UNP W5ZZF5
H	1327	LEU	-	expression tag	UNP W5ZZF5
H	1328	PHE	-	expression tag	UNP W5ZZF5
H	1329	GLN	-	expression tag	UNP W5ZZF5
I	506	PHE	LEU	conflict	UNP W5ZZF5
I	748	ALA	ARG	conflict	UNP W5ZZF5
I	751	GLY	ARG	conflict	UNP W5ZZF5
I	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
I	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
I	1292	GLY	-	expression tag	UNP W5ZZF5
I	1293	SER	-	expression tag	UNP W5ZZF5
I	1294	GLY	-	expression tag	UNP W5ZZF5
I	1295	TYR	-	expression tag	UNP W5ZZF5
I	1296	ILE	-	expression tag	UNP W5ZZF5
I	1297	PRO	-	expression tag	UNP W5ZZF5
I	1298	GLU	-	expression tag	UNP W5ZZF5
I	1299	ALA	-	expression tag	UNP W5ZZF5
I	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1301	ARG	-	expression tag	UNP W5ZZF5
I	1302	ASP	-	expression tag	UNP W5ZZF5
I	1303	GLY	-	expression tag	UNP W5ZZF5
I	1304	GLN	-	expression tag	UNP W5ZZF5
I	1305	ALA	-	expression tag	UNP W5ZZF5
I	1306	TYR	-	expression tag	UNP W5ZZF5
I	1307	VAL	-	expression tag	UNP W5ZZF5
I	1308	ARG	-	expression tag	UNP W5ZZF5
I	1309	LYS	-	expression tag	UNP W5ZZF5
I	1310	ASP	-	expression tag	UNP W5ZZF5
I	1311	GLY	-	expression tag	UNP W5ZZF5
I	1312	GLU	-	expression tag	UNP W5ZZF5
I	1313	TRP	-	expression tag	UNP W5ZZF5
I	1314	VAL	-	expression tag	UNP W5ZZF5
I	1315	LEU	-	expression tag	UNP W5ZZF5
I	1316	LEU	-	expression tag	UNP W5ZZF5
I	1317	SER	-	expression tag	UNP W5ZZF5
I	1318	THR	-	expression tag	UNP W5ZZF5
I	1319	PHE	-	expression tag	UNP W5ZZF5
I	1320	LEU	-	expression tag	UNP W5ZZF5
I	1321	GLY	-	expression tag	UNP W5ZZF5
I	1322	ARG	-	expression tag	UNP W5ZZF5
I	1323	SER	-	expression tag	UNP W5ZZF5
I	1324	LEU	-	expression tag	UNP W5ZZF5
I	1325	GLU	-	expression tag	UNP W5ZZF5
I	1326	VAL	-	expression tag	UNP W5ZZF5
I	1327	LEU	-	expression tag	UNP W5ZZF5
I	1328	PHE	-	expression tag	UNP W5ZZF5
I	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

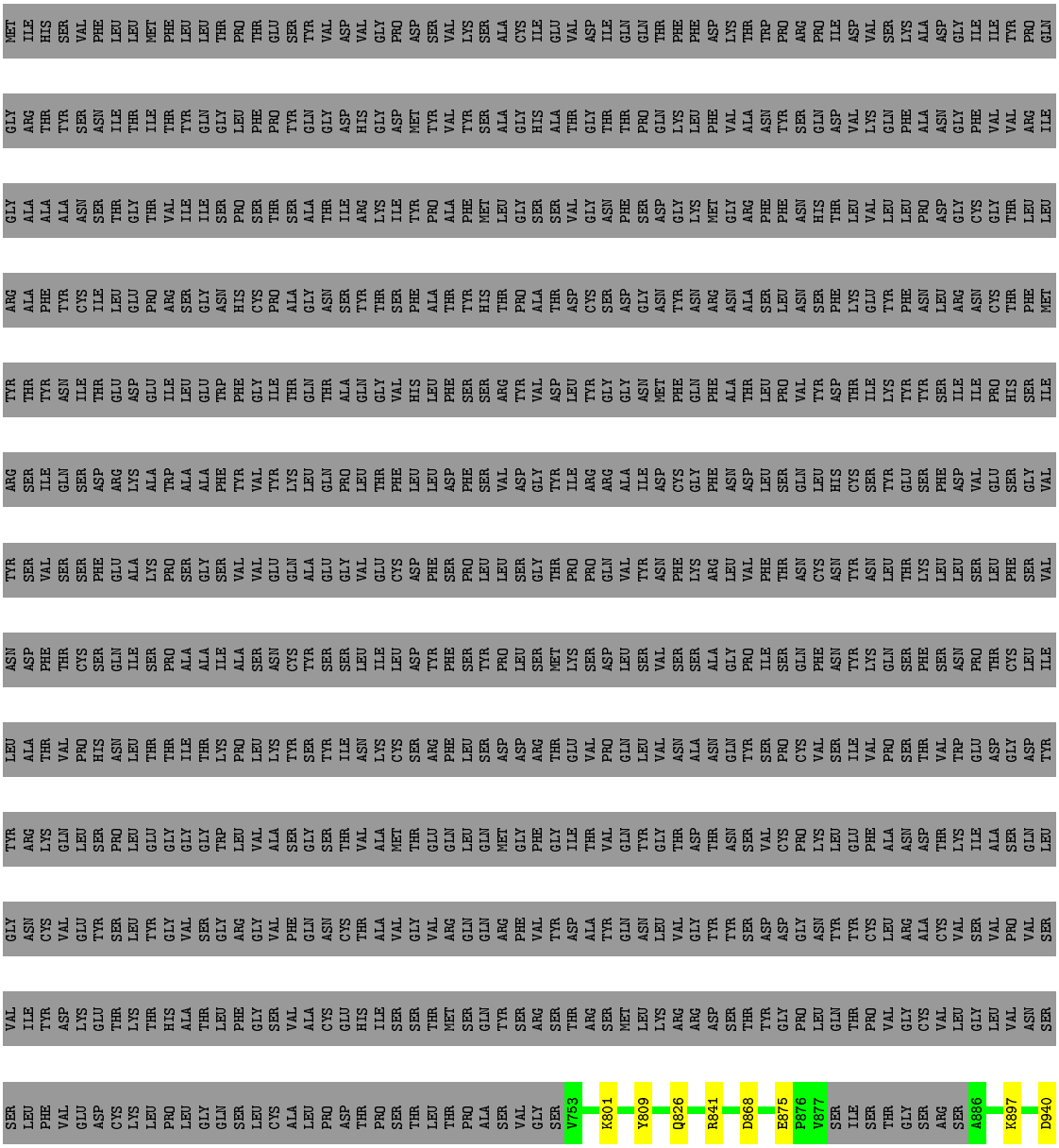
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total	C	N	O	S	0	0
			835	522	143	166	4		
3	F	111	Total	C	N	O	S	0	0
			835	522	143	166	4		

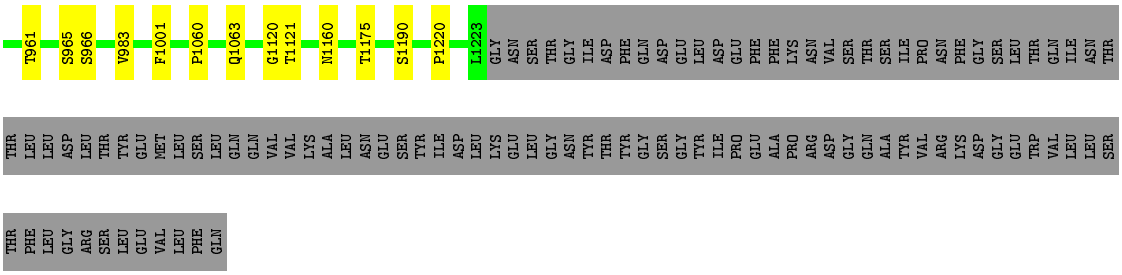
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: MERS S

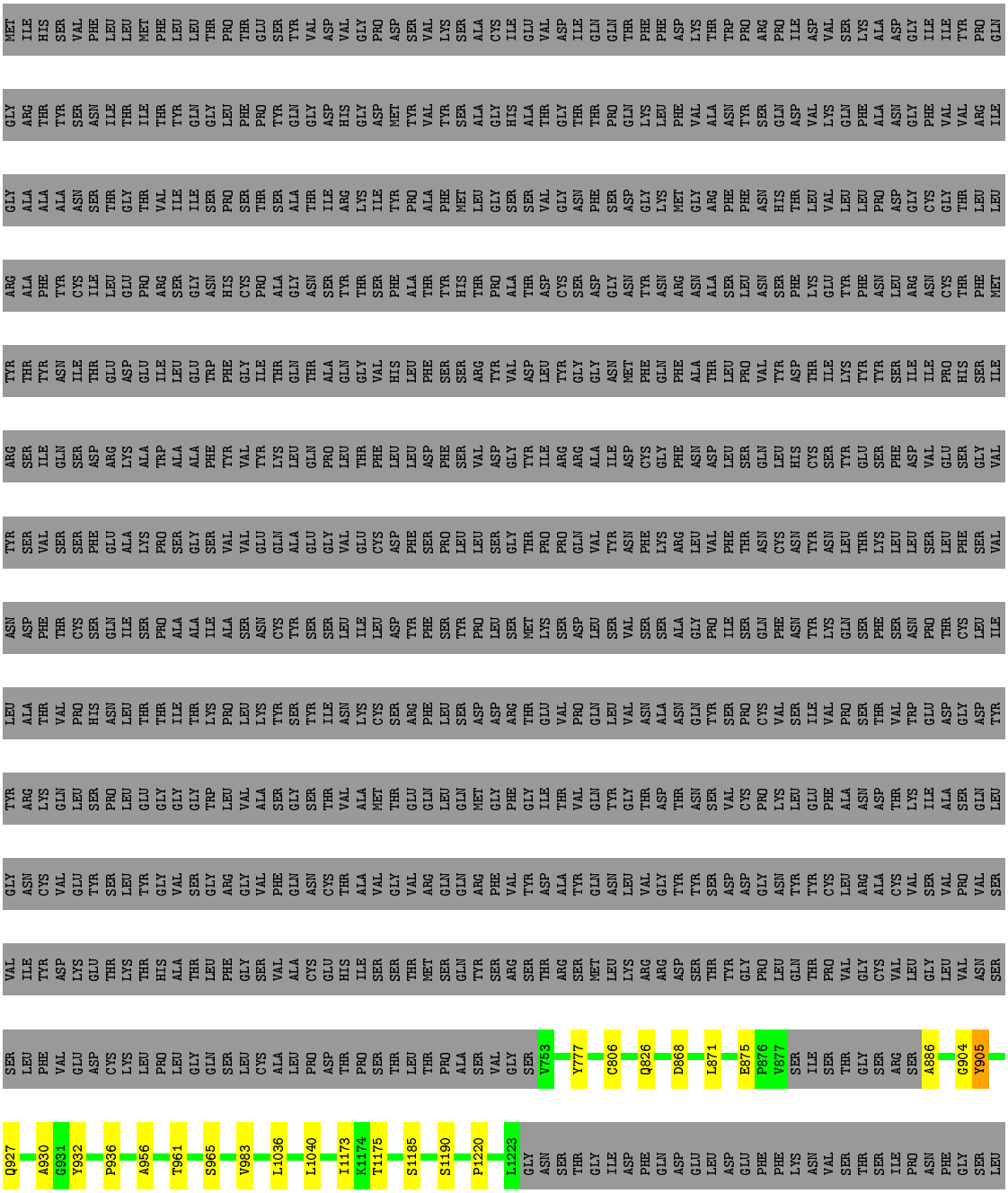
Chain A:



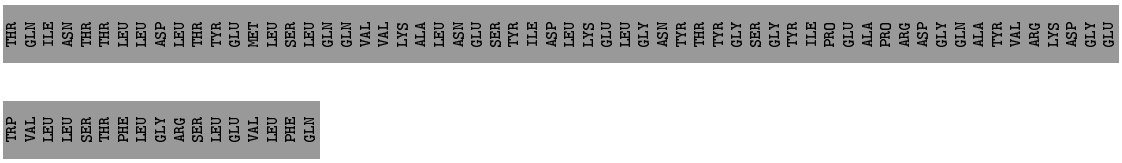


- Molecule 1: MERS S

Chain D:

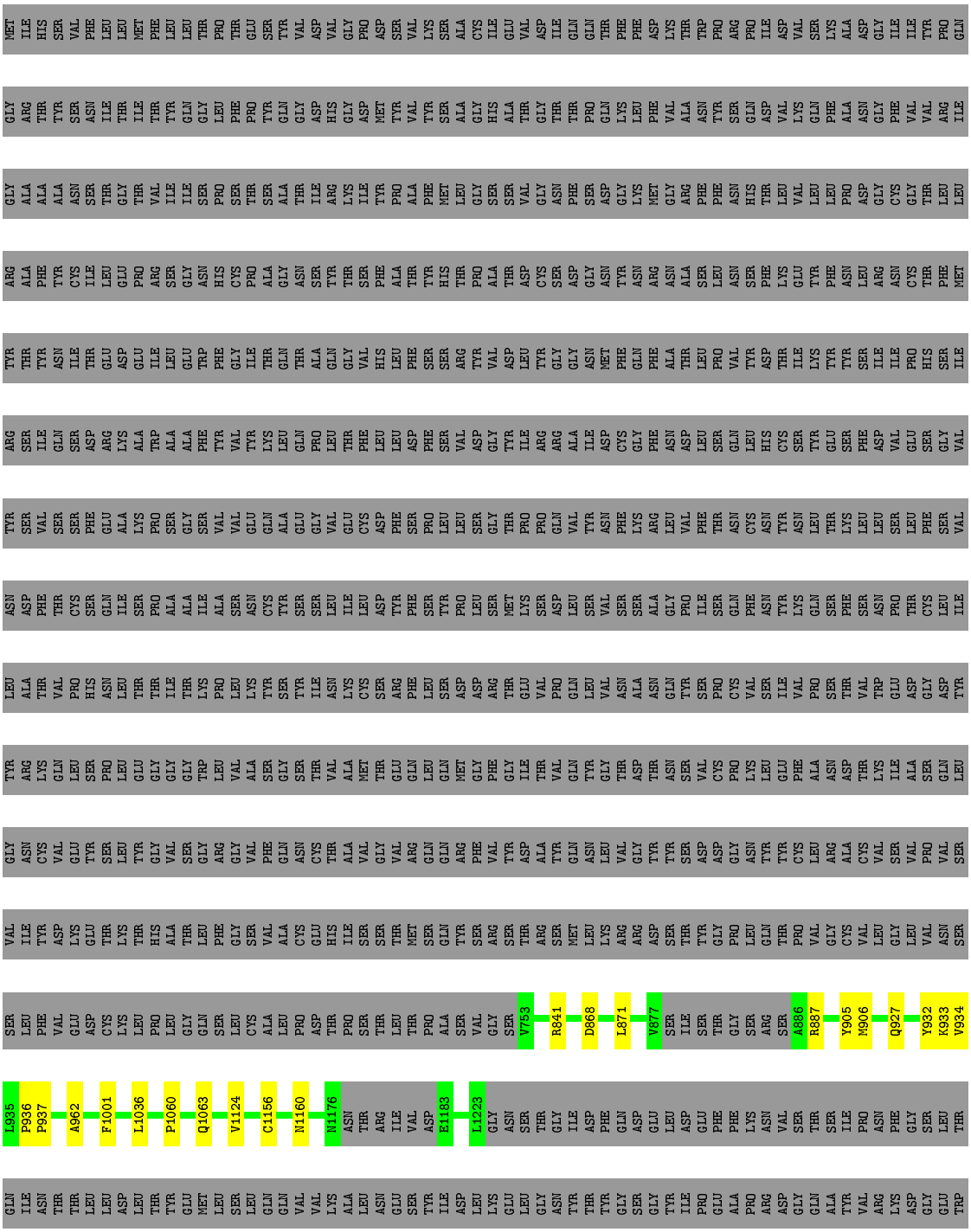


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



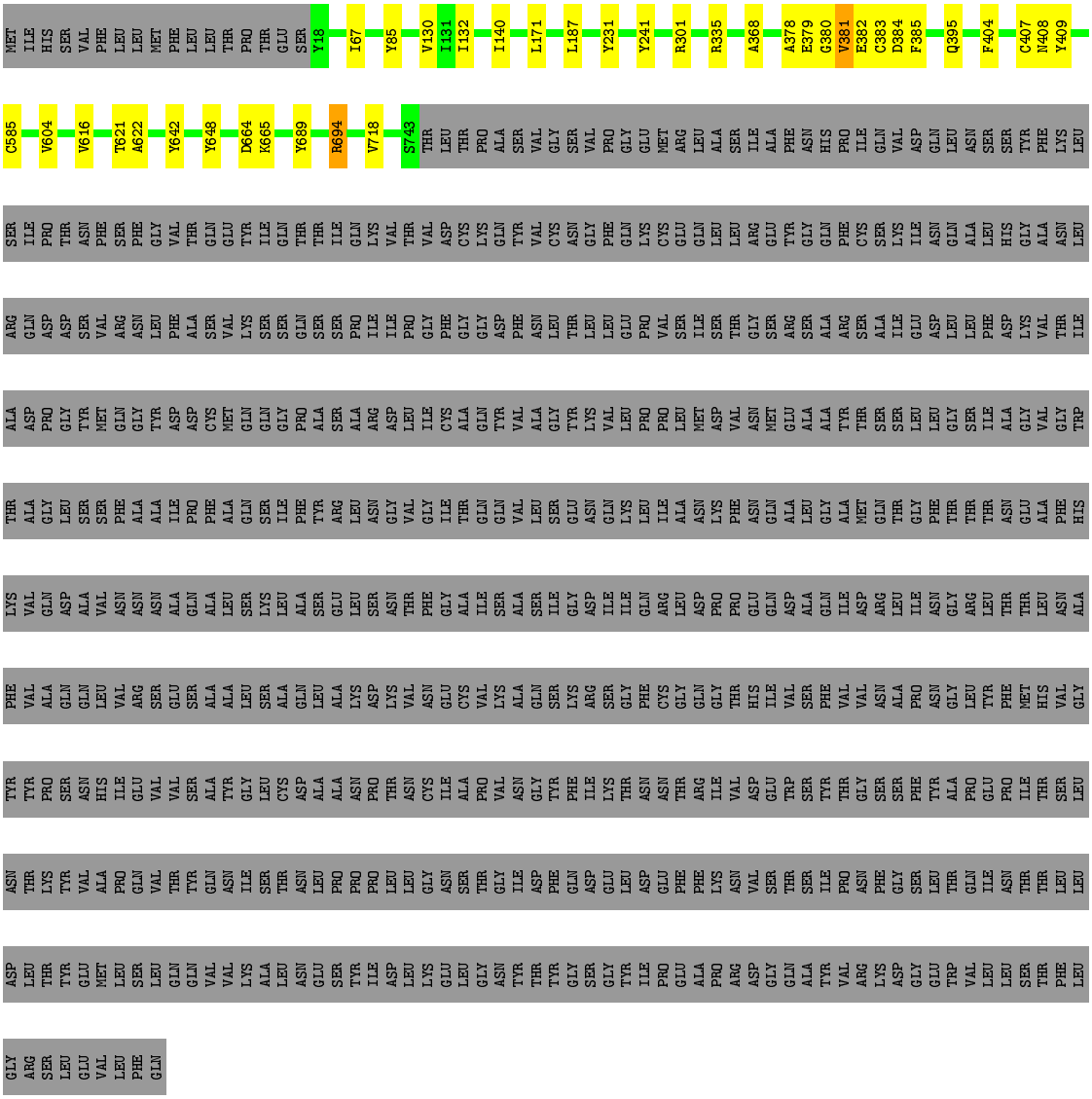
- Molecule 1: MERS S

Chain G:



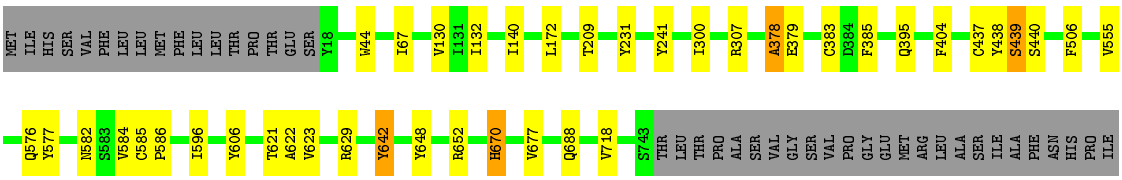
- Molecule 1: MERS S

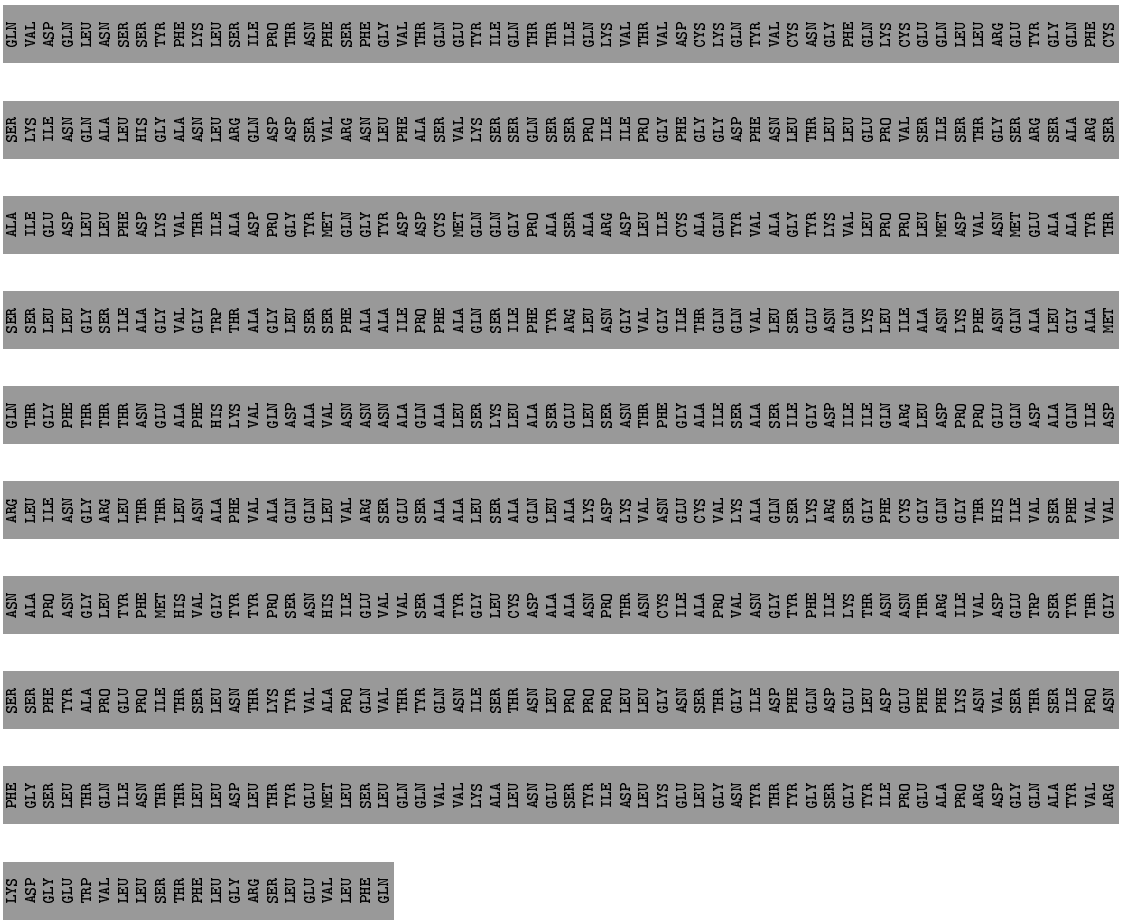
Chain H:



- Molecule 1: MERS S

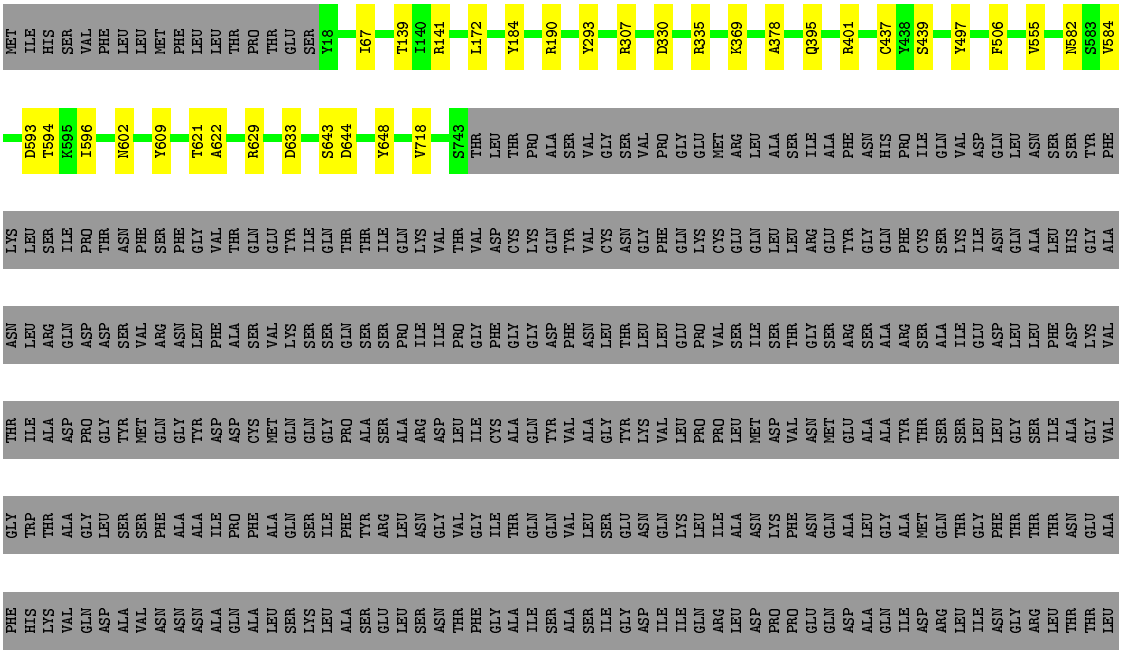
Chain I:

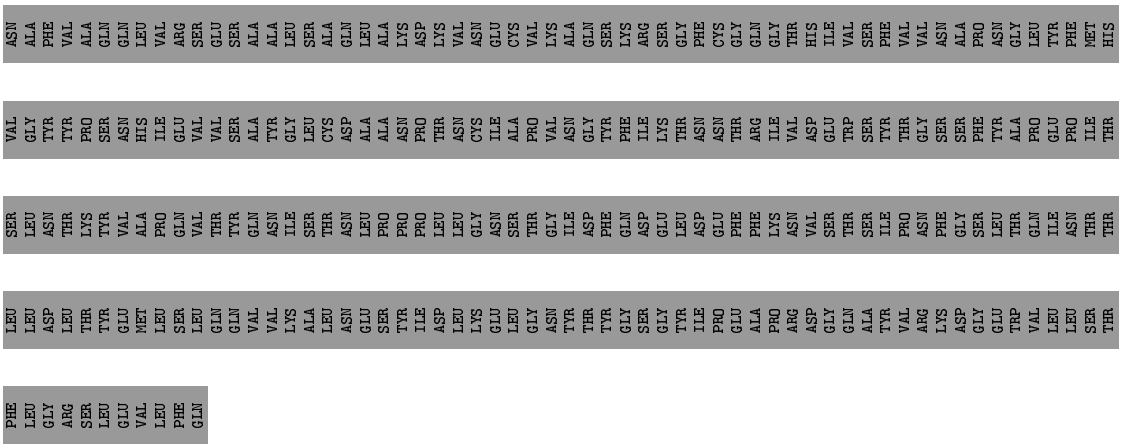




- Molecule 1: MERS S

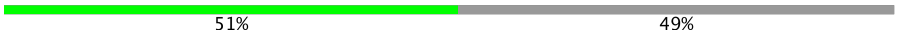
Chain J:

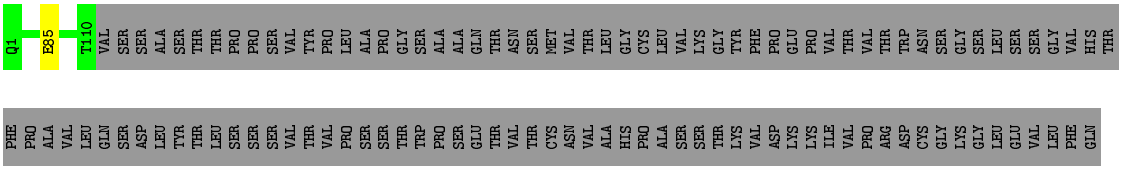




- Molecule 2: G4 VH

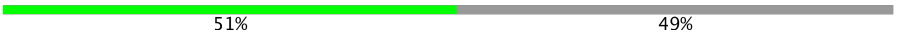
Chain B:

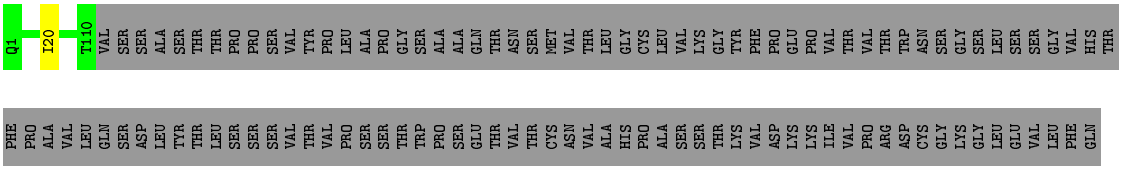




- Molecule 2: G4 VH

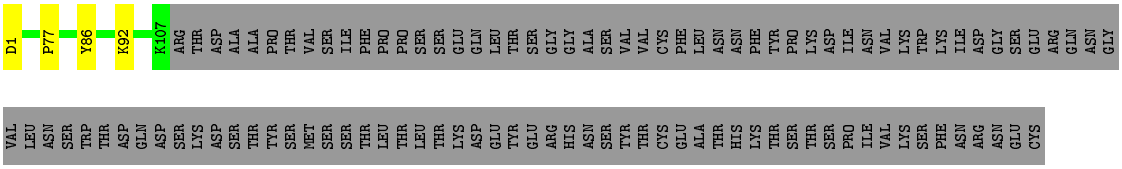
Chain E:





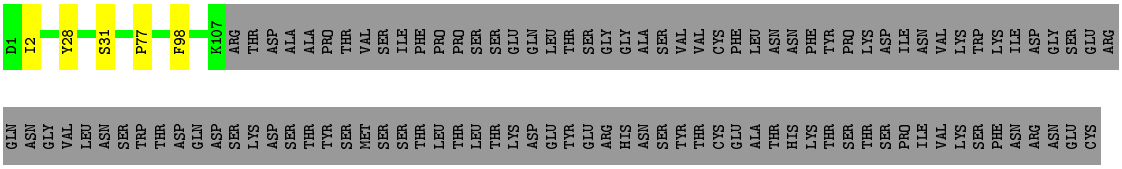
- Molecule 3: G4 VL

Chain C:



- Molecule 3: G4 VL

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8133	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.72	0/3618	0.81	1/4921 (0.0%)
1	D	0.72	0/3618	0.81	1/4921 (0.0%)
1	G	0.72	0/3568	0.82	4/4851 (0.1%)
1	H	0.72	0/5803	0.89	8/7901 (0.1%)
1	I	0.72	0/5803	0.89	5/7901 (0.1%)
1	J	0.73	0/5803	0.91	11/7901 (0.1%)
2	B	0.71	0/972	0.83	0/1317
2	E	0.74	0/972	0.84	0/1317
3	C	0.76	0/852	0.81	1/1153 (0.1%)
3	F	0.80	0/852	0.87	1/1153 (0.1%)
All	All	0.73	0/31861	0.86	32/43336 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	1156	CYS	O-C-N	-9.22	107.94	122.70
1	I	642	TYR	CB-CG-CD1	-7.73	116.36	121.00
1	J	584	VAL	C-N-CA	7.44	140.30	121.70
1	G	1156	CYS	CA-C-O	7.40	135.64	120.10
1	H	642	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	J	190	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	H	85	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	H	694	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	I	307	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	J	437	CYS	O-C-N	-6.07	112.99	122.70
1	I	241	TYR	CB-CG-CD2	-6.04	117.37	121.00
1	H	585	CYS	CA-CB-SG	5.92	124.66	114.00
1	H	694	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	H	231	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	H	335	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	J	307	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	J	190	ARG	NE-CZ-NH1	5.51	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	231	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	I	378	ALA	C-N-CA	5.50	135.44	121.70
1	G	887	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	241	TYR	CB-CG-CD2	-5.45	117.73	121.00
3	F	98	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	J	497	TYR	CB-CG-CD1	-5.27	117.84	121.00
3	C	86	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	G	868	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	184	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	D	868	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	868	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	293	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	J	335	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	J	609	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	J	401	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3545	0	3470	14	0
1	D	3545	0	3471	27	0
1	G	3496	0	3420	14	0
1	H	5658	0	5425	34	0
1	I	5658	0	5425	57	0
1	J	5658	0	5423	26	0
2	B	948	0	904	1	0
2	E	948	0	904	2	0
3	C	835	0	816	2	0
3	F	835	0	816	2	0
All	All	31126	0	30074	179	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 3.

All (179) 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:J:506:PHE:CE2	1:J:555:VAL:HG21	1.09	1.61
1:I:506:PHE:CE2	1:I:555:VAL:CG2	1.84	1.58
1:I:506:PHE:CE2	1:I:555:VAL:HG21	0.95	1.47
1:I:506:PHE:HE2	1:I:555:VAL:CG2	1.15	1.43
1:J:506:PHE:CE2	1:J:555:VAL:CG2	2.00	1.42
1:D:905:TYR:OH	1:D:936:PRO:CA	1.80	1.30
1:I:437:CYS:CB	1:I:584:VAL:O	1.80	1.27
1:D:905:TYR:OH	1:D:936:PRO:HA	1.26	1.23
1:I:506:PHE:CD2	1:I:555:VAL:HG21	1.75	1.21
1:I:437:CYS:CB	1:I:585:CYS:HA	1.72	1.17
1:I:506:PHE:CD2	1:I:555:VAL:CG2	2.28	1.15
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.82	1.15
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.43	1.14
1:I:437:CYS:HB3	1:I:585:CYS:HA	1.20	1.14
1:H:381:VAL:HG11	1:H:407:CYS:HA	1.28	1.10
1:I:437:CYS:HB2	1:I:584:VAL:O	0.89	1.06
1:J:621:THR:HG22	1:J:622:ALA:H	1.21	1.05
1:G:905:TYR:OH	1:G:934:VAL:O	1.75	1.03
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.42	0.99
1:J:621:THR:HG22	1:J:622:ALA:N	1.77	0.98
1:I:506:PHE:CD2	1:I:555:VAL:HG23	2.04	0.92
1:I:621:THR:O	1:I:648:TYR:HD2	1.53	0.90
1:H:384:ASP:O	1:H:404:PHE:CZ	2.24	0.90
1:J:621:THR:CG2	1:J:622:ALA:H	1.84	0.89
1:H:621:THR:O	1:H:648:TYR:HD2	1.55	0.89
1:J:621:THR:O	1:J:648:TYR:HD2	1.55	0.89
1:I:506:PHE:HE2	1:I:555:VAL:CB	1.87	0.88
1:D:927:GLN:HA	1:D:932:TYR:HB2	1.58	0.86
1:H:378:ALA:O	1:H:379:GLU:HG2	1.75	0.86
1:G:871:LEU:HG	1:G:871:LEU:O	1.75	0.85
1:I:621:THR:HG22	1:I:622:ALA:N	1.91	0.85
1:I:437:CYS:HB2	1:I:584:VAL:C	1.98	0.84
1:D:905:TYR:OH	1:D:936:PRO:N	2.12	0.82
1:H:381:VAL:CG1	1:H:407:CYS:HA	2.09	0.82
1:I:438:TYR:O	1:I:440:SER:N	2.14	0.80
1:D:871:LEU:HG	1:D:871:LEU:O	1.81	0.80
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.17	0.80
1:D:932:TYR:OH	1:D:1036:LEU:HB2	1.83	0.78
1:I:506:PHE:CE2	1:I:555:VAL:CB	2.63	0.77
1:H:384:ASP:O	1:H:404:PHE:HZ	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:621:THR:O	1:H:648:TYR:CD2	2.37	0.77
1:I:437:CYS:SG	1:I:585:CYS:CB	2.73	0.76
2:E:20:ILE:HD12	2:E:20:ILE:C	2.08	0.74
1:J:621:THR:O	1:J:648:TYR:CD2	2.42	0.73
1:A:983:VAL:O	1:A:1190:SER:OG	2.05	0.73
1:I:621:THR:HG22	1:I:622:ALA:H	1.53	0.73
1:I:621:THR:O	1:I:648:TYR:CD2	2.40	0.73
1:I:506:PHE:HD2	1:I:555:VAL:HG23	1.50	0.72
1:H:621:THR:HG22	1:H:622:ALA:N	2.06	0.70
1:I:621:THR:CG2	1:I:622:ALA:H	2.05	0.70
1:I:621:THR:CG2	1:I:622:ALA:N	2.55	0.69
1:I:437:CYS:CB	1:I:585:CYS:CA	2.63	0.69
1:D:983:VAL:O	1:D:1190:SER:OG	2.10	0.68
1:H:616:VAL:HG13	1:H:616:VAL:O	1.93	0.68
1:I:438:TYR:HB3	1:I:576:GLN:O	1.92	0.68
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.28	0.68
1:I:437:CYS:SG	1:I:585:CYS:HA	2.35	0.67
1:J:172:LEU:HD12	1:J:172:LEU:O	1.95	0.67
1:I:437:CYS:HG	1:I:585:CYS:HG	1.27	0.67
1:D:927:GLN:CA	1:D:932:TYR:HB2	2.24	0.66
2:E:20:ILE:HD12	2:E:20:ILE:O	1.96	0.66
1:D:905:TYR:HH	1:D:936:PRO:HA	1.55	0.65
1:I:437:CYS:HB3	1:I:586:PRO:HD3	1.79	0.65
1:J:506:PHE:HE2	1:J:555:VAL:HG22	1.53	0.65
1:G:927:GLN:HG2	1:G:932:TYR:HB2	1.79	0.63
1:H:384:ASP:O	1:H:404:PHE:CE2	2.50	0.63
1:G:932:TYR:OH	1:G:1036:LEU:HB2	1.98	0.62
1:I:172:LEU:HD12	1:I:172:LEU:O	2.00	0.62
1:D:927:GLN:HG3	1:D:932:TYR:HB3	1.81	0.62
1:J:506:PHE:HE2	1:J:555:VAL:HG21	0.80	0.61
1:G:932:TYR:OH	1:G:1036:LEU:CB	2.49	0.60
1:I:437:CYS:SG	1:I:585:CYS:CA	2.89	0.60
1:D:905:TYR:OH	1:D:936:PRO:CB	2.49	0.60
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.85	0.59
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.84	0.59
1:H:381:VAL:O	1:H:382:GLU:HB3	2.03	0.59
1:D:905:TYR:CZ	1:D:936:PRO:HA	2.31	0.59
1:I:67:ILE:HG13	1:I:67:ILE:O	2.03	0.59
2:B:85:GLU:N	2:B:85:GLU:OE1	2.35	0.58
1:H:385:PHE:CE2	1:H:404:PHE:CE1	2.92	0.57
1:H:378:ALA:C	1:H:379:GLU:HG2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:GLU:HA	1:H:408:ASN:O	2.04	0.57
1:J:67:ILE:O	1:J:67:ILE:HG13	2.05	0.57
1:H:621:THR:CG2	1:H:622:ALA:N	2.67	0.56
1:D:932:TYR:OH	1:D:1036:LEU:CB	2.53	0.56
1:D:1175:THR:HG23	1:D:1175:THR:O	2.05	0.56
1:I:383:CYS:HB2	1:I:385:PHE:CE1	2.41	0.56
1:H:604:VAL:O	1:H:604:VAL:HG23	2.07	0.55
1:I:383:CYS:CB	1:I:385:PHE:CE1	2.91	0.54
1:A:1175:THR:HG23	1:A:1175:THR:O	2.08	0.54
1:A:897:LYS:HA	1:A:897:LYS:HE2	1.90	0.53
3:F:28:TYR:CD1	3:F:28:TYR:N	2.71	0.53
1:D:927:GLN:HG3	1:D:932:TYR:CB	2.38	0.53
1:I:438:TYR:C	1:I:440:SER:N	2.61	0.53
1:I:437:CYS:SG	1:I:584:VAL:O	2.67	0.53
1:H:395:GLN:OE1	1:H:395:GLN:HA	2.11	0.51
1:H:67:ILE:O	1:H:67:ILE:HG13	2.10	0.50
1:I:438:TYR:O	1:I:439:SER:C	2.50	0.50
1:G:932:TYR:N	1:G:932:TYR:CD1	2.78	0.50
1:I:623:VAL:O	1:I:642:TYR:OH	2.27	0.49
1:I:438:TYR:HB3	1:I:576:GLN:C	2.33	0.49
1:J:369:LYS:O	1:J:369:LYS:HG2	2.12	0.49
3:C:1:ASP:C	3:C:1:ASP:OD1	2.52	0.49
1:I:385:PHE:CE2	1:I:404:PHE:CE1	3.01	0.48
1:H:616:VAL:O	1:H:616:VAL:CG1	2.59	0.48
1:D:777:TYR:N	1:D:777:TYR:CD2	2.81	0.48
1:A:875:GLU:O	1:A:875:GLU:HG2	2.13	0.48
1:G:906:MET:HG2	1:G:906:MET:O	2.14	0.48
1:H:621:THR:CG2	1:H:622:ALA:H	2.26	0.47
1:G:933:LYS:O	1:G:934:VAL:C	2.52	0.47
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.14	0.47
1:H:664:ASP:C	1:H:664:ASP:OD1	2.53	0.47
1:A:875:GLU:OE1	1:A:875:GLU:N	2.38	0.47
1:J:139:THR:OG1	1:J:141:ARG:NH1	2.48	0.47
1:H:301:ARG:O	1:H:301:ARG:HG2	2.14	0.46
1:G:1001:PHE:CD2	1:G:1001:PHE:C	2.89	0.46
1:J:439:SER:HA	1:J:582:ASN:HA	1.98	0.46
1:H:171:LEU:HD23	1:H:171:LEU:C	2.36	0.46
1:D:904:GLY:O	1:D:905:TYR:HB2	2.16	0.45
1:A:809:TYR:CD2	1:A:809:TYR:C	2.90	0.45
1:I:130:VAL:O	1:I:130:VAL:HG12	2.16	0.45
1:A:1001:PHE:C	1:A:1001:PHE:CD2	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:GLU:HB3	1:D:886:ALA:HB3	1.99	0.45
1:I:606:TYR:C	1:I:606:TYR:CD1	2.90	0.45
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	1.98	0.45
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	1.98	0.44
1:J:621:THR:CG2	1:J:622:ALA:N	2.45	0.44
1:I:300:ILE:HD12	1:I:300:ILE:N	2.32	0.44
1:I:677:VAL:O	1:I:677:VAL:HG22	2.16	0.44
1:I:130:VAL:O	1:I:130:VAL:CG1	2.66	0.44
1:I:438:TYR:HD2	1:I:577:TYR:HB2	1.83	0.44
1:I:596:ILE:C	1:I:596:ILE:HD12	2.38	0.44
1:I:670:HIS:CD2	1:I:670:HIS:N	2.84	0.44
1:H:694:ARG:HA	1:H:694:ARG:NE	2.33	0.43
1:I:395:GLN:OE1	1:I:395:GLN:HA	2.17	0.43
1:D:1175:THR:CG2	1:D:1175:THR:O	2.67	0.43
1:D:905:TYR:CE1	1:D:936:PRO:HB3	2.54	0.43
1:I:209:THR:O	1:I:209:THR:HG22	2.18	0.43
1:I:439:SER:HA	1:I:582:ASN:HA	2.00	0.43
1:A:801:LYS:HE3	1:A:801:LYS:HB2	1.85	0.43
3:F:2:ILE:N	3:F:2:ILE:HD12	2.33	0.43
1:I:132:ILE:HA	1:I:132:ILE:HD12	1.73	0.43
1:I:652:ARG:HA	1:I:652:ARG:NE	2.34	0.43
1:I:438:TYR:CB	1:I:576:GLN:O	2.63	0.43
1:A:826:GLN:OE1	1:A:826:GLN:N	2.32	0.43
1:J:643:SER:OG	1:J:644:ASP:N	2.50	0.42
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.58	0.42
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.57	0.42
1:G:1124:VAL:HG13	1:G:1124:VAL:O	2.19	0.42
1:H:383:CYS:HB3	1:H:385:PHE:CE1	2.55	0.42
1:H:694:ARG:HA	1:H:694:ARG:HE	1.85	0.42
1:I:383:CYS:HB3	1:I:385:PHE:CE1	2.54	0.42
1:J:172:LEU:C	1:J:172:LEU:HD12	2.39	0.42
1:I:688:GLN:OE1	1:I:688:GLN:HA	2.20	0.42
1:H:621:THR:HG22	1:H:622:ALA:H	1.80	0.42
1:D:806:CYS:SG	1:D:806:CYS:O	2.77	0.41
1:G:841:ARG:HA	1:G:841:ARG:NE	2.34	0.41
1:D:930:ALA:HB2	1:D:1040:LEU:HD11	2.01	0.41
1:I:140:ILE:HD13	1:I:140:ILE:HG21	1.77	0.41
1:I:378:ALA:HB1	1:I:379:GLU:HA	2.03	0.41
1:J:330:ASP:OD1	1:J:330:ASP:C	2.58	0.41
1:A:965:SER:OG	1:A:966:SER:N	2.52	0.41
1:H:383:CYS:SG	1:H:409:TYR:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:593:ASP:N	1:J:594:THR:HA	2.35	0.41
1:J:506:PHE:HD2	1:J:555:VAL:HG23	1.81	0.41
1:A:1120:GLY:O	1:A:1121:THR:OG1	2.30	0.41
3:C:92:LYS:C	3:C:92:LYS:HD3	2.41	0.41
1:D:826:GLN:OE1	1:D:826:GLN:N	2.28	0.41
1:H:665:LYS:C	1:H:665:LYS:HD3	2.41	0.41
1:I:506:PHE:HE2	1:I:555:VAL:CG1	2.31	0.41
1:H:130:VAL:O	1:H:130:VAL:HG12	2.21	0.41
1:H:140:ILE:HG21	1:H:140:ILE:HD13	1.83	0.41
1:H:689:TYR:CD1	1:H:689:TYR:C	2.94	0.41
1:A:841:ARG:NE	1:A:841:ARG:HA	2.35	0.41
1:G:936:PRO:HA	1:G:937:PRO:HD3	1.96	0.40
1:J:633:ASP:C	1:J:633:ASP:OD1	2.58	0.40
1:H:187:LEU:HD23	1:H:187:LEU:HA	1.87	0.40
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.22	0.40
1:H:132:ILE:HD12	1:H:132:ILE:HA	1.87	0.40

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	459/1329 (34%)	441 (96%)	15 (3%)	3 (1%)	25 68
1	D	459/1329 (34%)	440 (96%)	14 (3%)	5 (1%)	17 60
1	G	451/1329 (34%)	433 (96%)	17 (4%)	1 (0%)	51 85
1	H	724/1329 (54%)	693 (96%)	27 (4%)	4 (1%)	28 70
1	I	724/1329 (54%)	691 (95%)	29 (4%)	4 (1%)	28 70
1	J	724/1329 (54%)	695 (96%)	24 (3%)	5 (1%)	25 68
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	C	109/218 (50%)	103 (94%)	5 (5%)	1 (1%)	20	63
3	F	109/218 (50%)	105 (96%)	2 (2%)	2 (2%)	10	49
All	All	3993/8876 (45%)	3831 (96%)	137 (3%)	25 (1%)	33	70

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	THR
1	G	962	ALA
1	H	381	VAL
1	I	439	SER
1	J	378	ALA
1	A	940	ASP
1	D	961	THR
1	D	965	SER
1	H	718	VAL
1	I	718	VAL
1	J	602	ASN
1	J	718	VAL
3	C	77	PRO
1	D	905	TYR
1	A	1220	PRO
1	D	1220	PRO
3	F	31	SER
3	F	77	PRO
1	J	596	ILE
1	J	629	ARG
1	D	956	ALA
1	H	368	ALA
1	H	380	GLY
1	I	629	ARG
1	I	44	TRP

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 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	388/1148 (34%)	388 (100%)	0	100 100
1	D	388/1148 (34%)	388 (100%)	0	100 100
1	G	382/1148 (33%)	382 (100%)	0	100 100
1	H	635/1148 (55%)	635 (100%)	0	100 100
1	I	635/1148 (55%)	634 (100%)	1 (0%)	94 96
1	J	635/1148 (55%)	635 (100%)	0	100 100
2	B	102/202 (50%)	102 (100%)	0	100 100
2	E	102/202 (50%)	102 (100%)	0	100 100
3	C	93/192 (48%)	93 (100%)	0	100 100
3	F	93/192 (48%)	93 (100%)	0	100 100
All	All	3453/7676 (45%)	3452 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	670	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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.