



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J3S
EMDB ID : EMD-5608
Title : Structural dynamics of the MecA-ClpC complex revealed by cryo-EM
Authors : Liu, J.; Mei, Z.; Li, N.; Qi, Y.; Xu, Y.; Shi, Y.; Wang, F.; Lei, J.; Gao, N.
Deposited on : 2013-04-18
Resolution : 11.00 Å(reported)
Based on PDB ID : 3PXI

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>

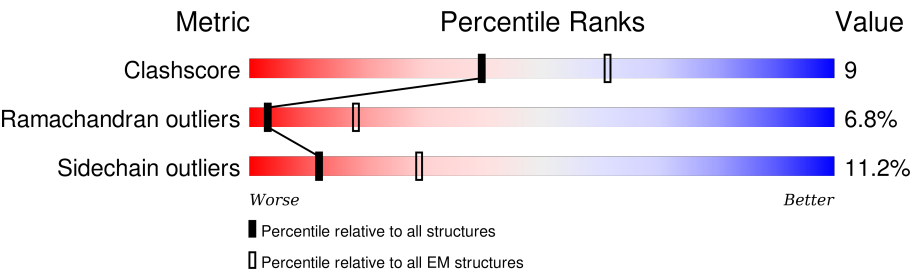
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 11.00 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	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	1	218	
1	2	218	
1	3	218	
1	4	218	
1	5	218	
1	6	218	
2	A	810	
2	B	810	
2	C	810	

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Mol	Chain	Length	Quality of chain
2	D	810	<div><div></div><div>65%28%5%<div><div></div><div></div><div></div></div></div></div>
2	E	810	<div><div></div><div>69%22%6%<div><div></div><div></div><div></div></div></div></div>
2	F	810	<div><div></div><div>68%25%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41862 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 Adapter protein MecA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	2	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	3	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	4	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	5	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	6	94	Total	C	N	O	S	0	0
			777	498	123	154	2		

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	B	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	C	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	D	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	E	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	F	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

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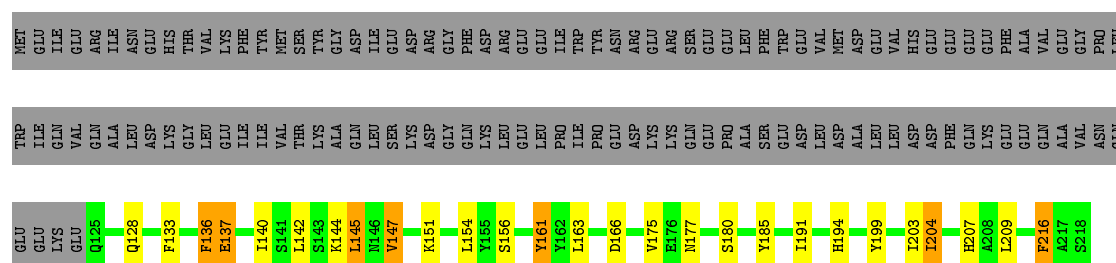
Chain	Residue	Modelled	Actual	Comment	Reference
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
E	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
F	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

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. 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.

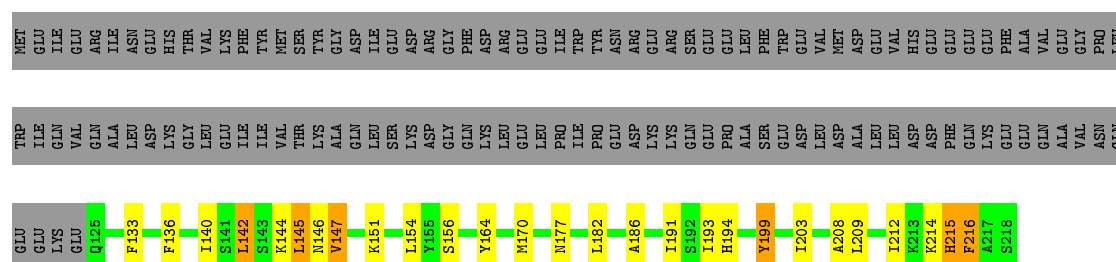
• Molecule 1: Adapter protein MecA 1

Chain 1: 



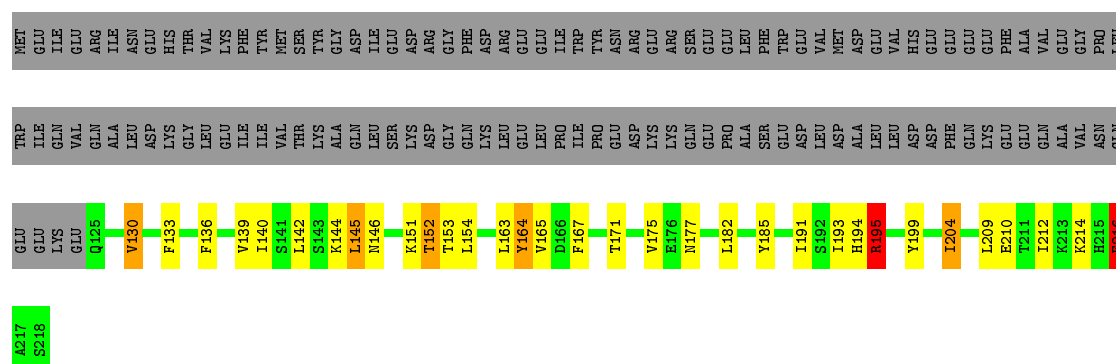
• Molecule 1: Adapter protein MecA 1

Chain 2: 



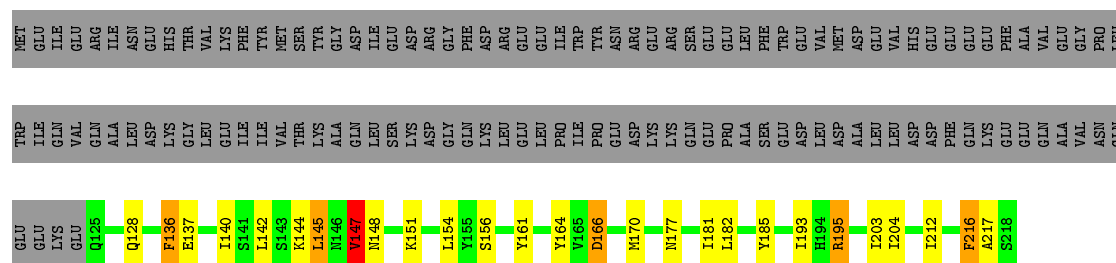
• Molecule 1: Adapter protein MecA 1

Chain 3: 



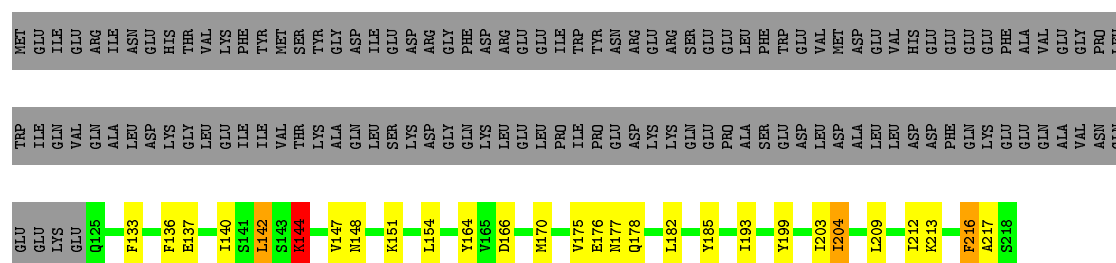
- Molecule 1: Adapter protein MecA 1

Chain 4: 



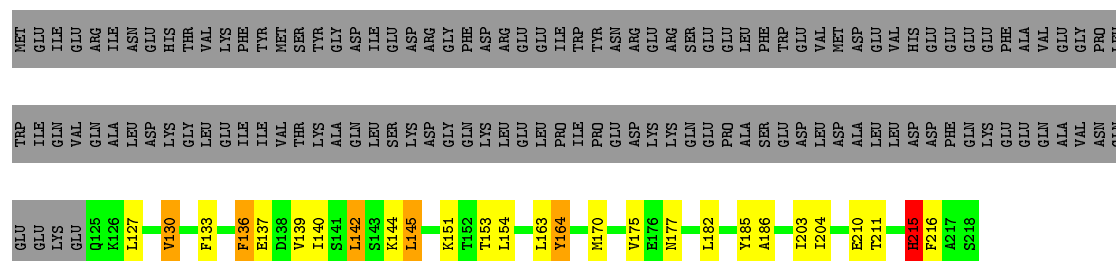
- Molecule 1: Adapter protein MecA 1

Chain 5: 



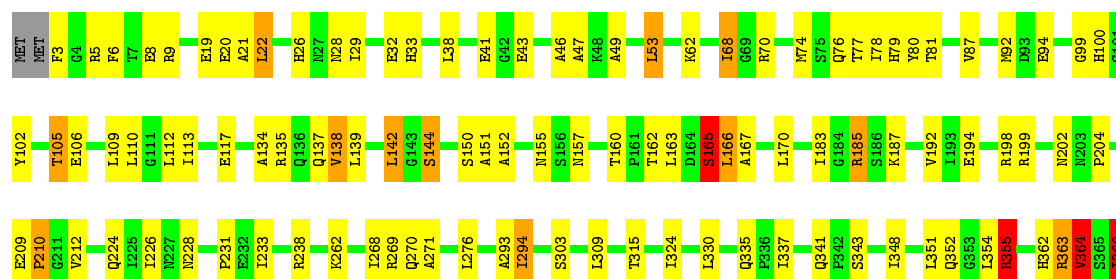
- Molecule 1: Adapter protein MecA 1

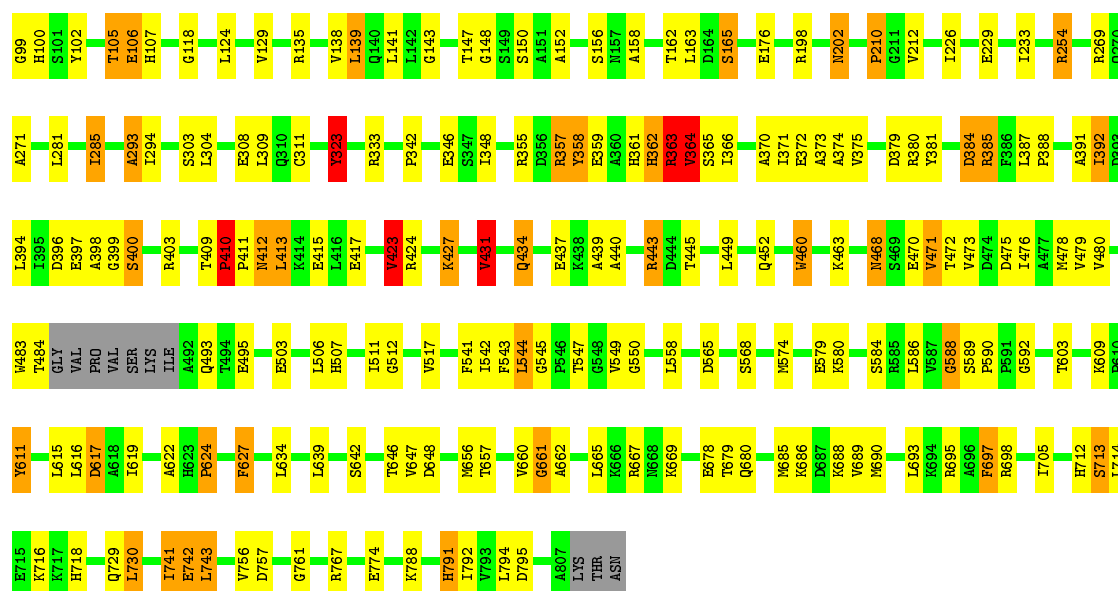
Chain 6: 



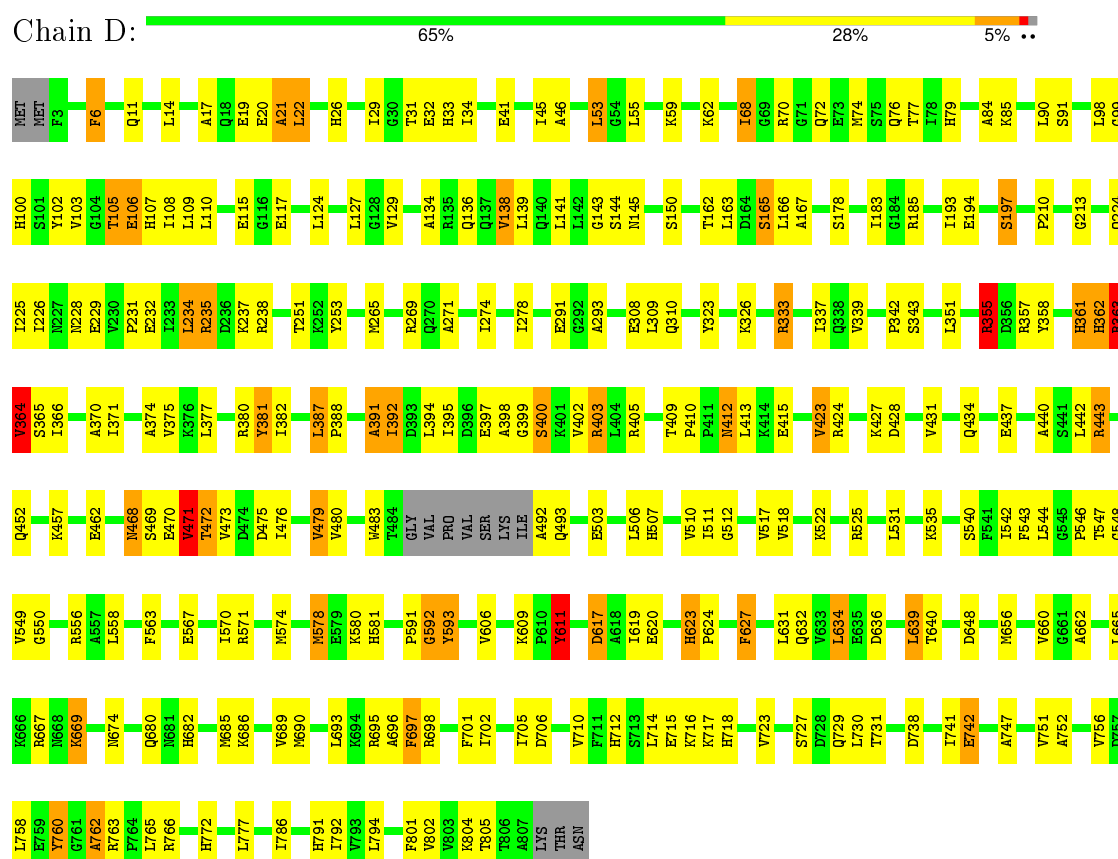
- Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain A: 



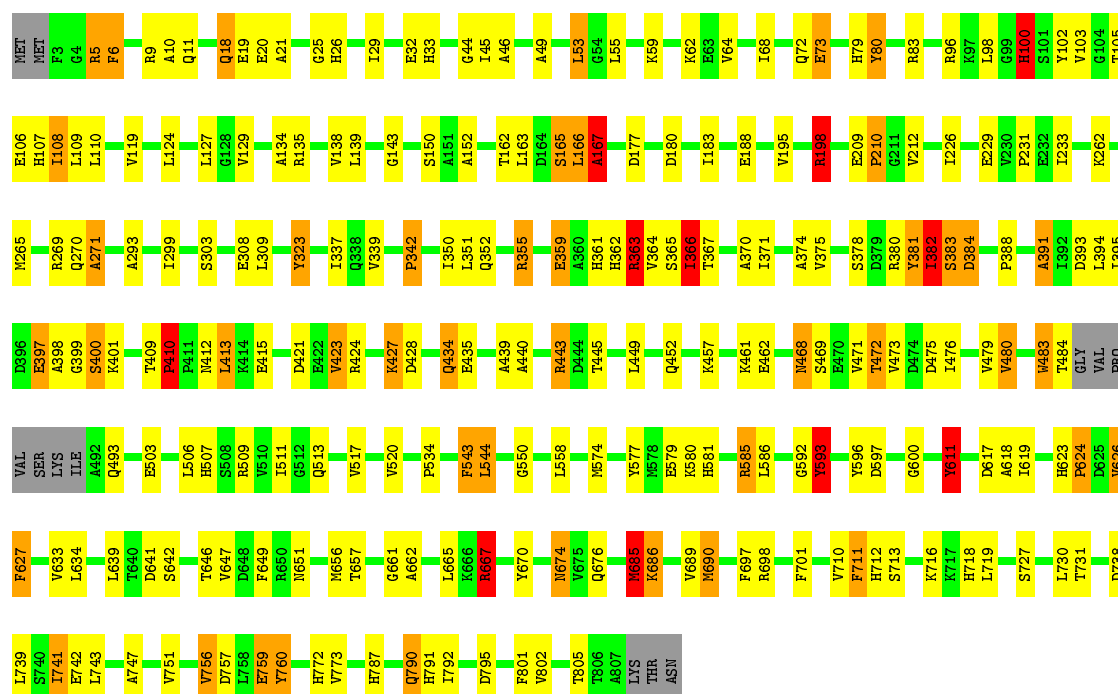


• Molecule 2: Negative regulator of genetic competence ClpC/MecB



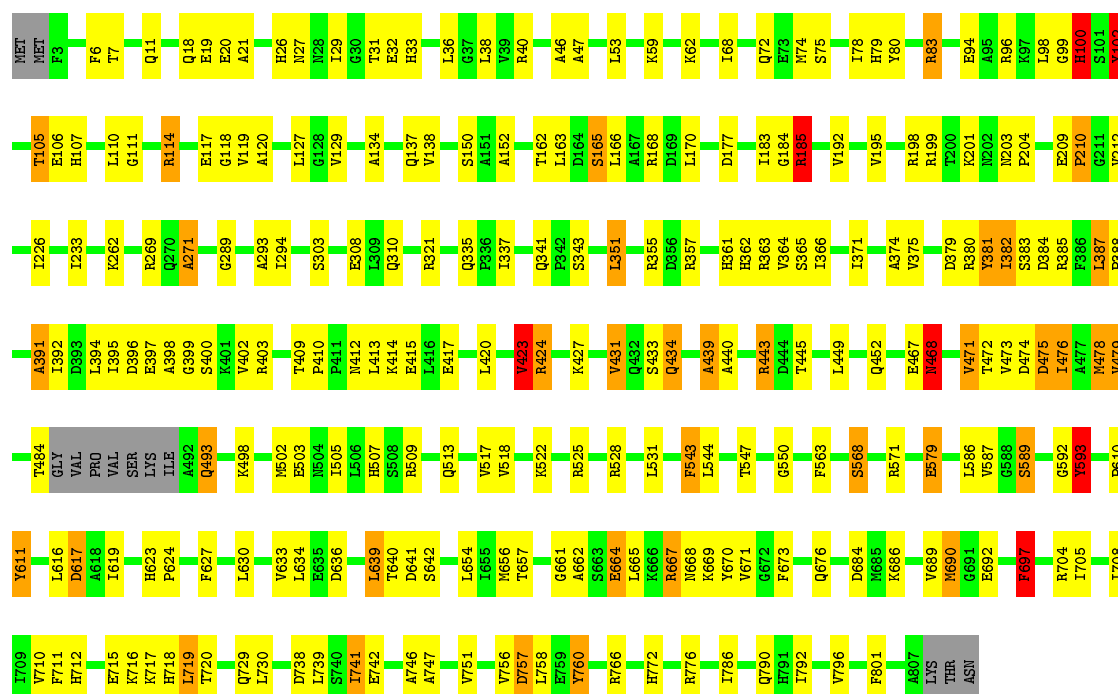
• Molecule 2: Negative regulator of genetic competence ClpC/MecB





- Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain F: 68% 25%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	41902	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each defocus group on 3D level	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI Eagle 4k*4k CCD	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	1	0.98	0/791	1.31	4/1064 (0.4%)
1	2	0.97	0/791	1.28	3/1064 (0.3%)
1	3	0.97	0/791	1.34	5/1064 (0.5%)
1	4	0.99	0/791	1.26	3/1064 (0.3%)
1	5	0.96	0/791	1.29	4/1064 (0.4%)
1	6	0.99	0/791	1.36	5/1064 (0.5%)
2	A	1.00	0/6269	1.26	27/8441 (0.3%)
2	B	1.00	0/6269	1.30	32/8441 (0.4%)
2	C	0.99	0/6269	1.27	28/8441 (0.3%)
2	D	1.00	0/6269	1.28	29/8441 (0.3%)
2	E	0.99	0/6269	1.29	36/8441 (0.4%)
2	F	1.01	0/6269	1.28	24/8441 (0.3%)
All	All	1.00	0/42360	1.28	200/57030 (0.4%)

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	1	0	1
1	2	0	1
1	3	0	4
1	4	0	1
1	5	0	1
1	6	0	2
2	A	0	19
2	B	0	20
2	C	0	12
2	D	0	17
2	E	0	15
2	F	0	14
All	All	0	107

There are no bond length outliers.

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	593	TYR	CB-CG-CD2	9.71	126.83	121.00
2	F	593	TYR	CB-CG-CD1	-8.53	115.88	121.00
2	E	167	ALA	N-CA-CB	8.31	121.74	110.10
2	C	588	GLY	N-CA-C	-8.22	92.55	113.10
2	E	611	TYR	CB-CG-CD2	-7.59	116.44	121.00

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	161	TYR	Sidechain
1	2	199	TYR	Sidechain
1	3	164	TYR	Sidechain
1	3	185	TYR	Sidechain
1	3	194	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	777	0	758	17	0
1	2	777	0	758	15	0
1	3	777	0	758	20	0
1	4	777	0	758	13	0
1	5	777	0	758	14	0
1	6	777	0	758	12	0
2	A	6200	0	6290	116	0
2	B	6200	0	6290	133	0
2	C	6200	0	6290	110	0
2	D	6200	0	6290	137	0
2	E	6200	0	6290	116	0
2	F	6200	0	6290	119	0
All	All	41862	0	42288	771	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 9.

The worst 5 of 771 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)
2:A:619:ILE:CD1	2:A:656:MET:HB3	1.24	1.66
2:A:619:ILE:CD1	2:A:656:MET:CB	2.18	1.21
2:F:619:ILE:HD12	2:F:656:MET:HB3	1.23	1.21
2:E:619:ILE:CD1	2:E:656:MET:HB3	1.69	1.20
2:F:619:ILE:CG2	2:F:627:PHE:CZ	2.27	1.18

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	1	92/218 (42%)	78 (85%)	8 (9%)	6 (6%)	1	25
1	2	92/218 (42%)	78 (85%)	9 (10%)	5 (5%)	2	29
1	3	92/218 (42%)	74 (80%)	12 (13%)	6 (6%)	1	25
1	4	92/218 (42%)	79 (86%)	8 (9%)	5 (5%)	2	29
1	5	92/218 (42%)	76 (83%)	12 (13%)	4 (4%)	3	34
1	6	92/218 (42%)	76 (83%)	13 (14%)	3 (3%)	5	40
2	A	794/810 (98%)	627 (79%)	109 (14%)	58 (7%)	1	21
2	B	794/810 (98%)	625 (79%)	117 (15%)	52 (6%)	1	25
2	C	794/810 (98%)	623 (78%)	118 (15%)	53 (7%)	1	24
2	D	794/810 (98%)	614 (77%)	125 (16%)	55 (7%)	1	23
2	E	794/810 (98%)	629 (79%)	107 (14%)	58 (7%)	1	21
2	F	794/810 (98%)	628 (79%)	112 (14%)	54 (7%)	1	23
All	All	5316/6168 (86%)	4207 (79%)	750 (14%)	359 (7%)	3	23

5 of 359 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	2	145	LEU
1	2	147	VAL
1	3	145	LEU
1	3	146	ASN

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	1	88/201 (44%)	80 (91%)	8 (9%)	12	43
1	2	88/201 (44%)	79 (90%)	9 (10%)	9	37
1	3	88/201 (44%)	79 (90%)	9 (10%)	9	37
1	4	88/201 (44%)	81 (92%)	7 (8%)	15	50
1	5	88/201 (44%)	80 (91%)	8 (9%)	12	43
1	6	88/201 (44%)	81 (92%)	7 (8%)	15	50
2	A	667/686 (97%)	584 (88%)	83 (12%)	6	30
2	B	667/686 (97%)	585 (88%)	82 (12%)	6	30
2	C	667/686 (97%)	591 (89%)	76 (11%)	7	33
2	D	667/686 (97%)	589 (88%)	78 (12%)	7	32
2	E	667/686 (97%)	597 (90%)	70 (10%)	8	36
2	F	667/686 (97%)	597 (90%)	70 (10%)	8	36
All	All	4530/5322 (85%)	4023 (89%)	507 (11%)	12	33

5 of 507 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	135	ARG
2	C	729	GLN
2	F	415	GLU
2	C	308	GLU

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Mol	Chain	Res	Type
2	C	452	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	504	ASN
2	D	100	HIS
2	F	681	ASN
2	C	507	HIS
2	D	26	HIS

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.