



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 11:29 AM EDT

PDB ID : 5A1W  
EMDB ID: : EMD-2987  
Title : The structure of the COPI coat linkage II  
Authors : Dodonova, S.O.; Diestelkoetter-Bachert, P.; von Appen, A.; Hagen, W.J.H.;  
Beck, R.; Beck, M.; Wieland, F.; Briggs, J.A.G.  
Deposited on : unknown  
Resolution : 18.00 Å(reported)

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

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

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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-20029824

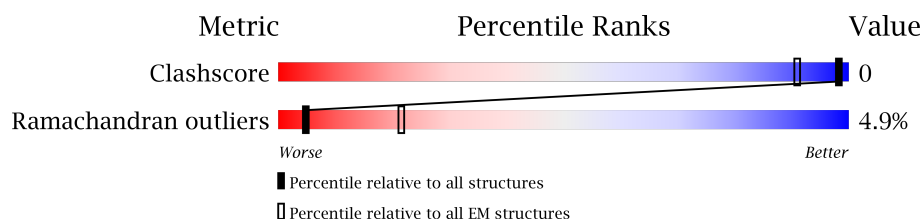
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 18.00 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

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	181	 88% 12%
1	B	181	 88% 12%
2	C	1262	 59% 5% 36%
3	D	905	 80% 9% 11%
4	E	874	 58% . . 37%
5	F	177	 75% . 21%
6	G	968	 73% 10% . 16%
7	H	511	 70% . 26%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15258 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 ADP-RIBOSYLATION FACTOR 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	159	Total	C	N	O	0	0
			636	318	159	159		
1	B	159	Total	C	N	O	0	0
			636	318	159	159		

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	813	Total	C	N	O	0	0
			3251	1626	813	812		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	LEU	-	expression tag	UNP Q8CIE6
C	1226	GLU	-	expression tag	UNP Q8CIE6
C	1227	VAL	-	expression tag	UNP Q8CIE6
C	1228	LEU	-	expression tag	UNP Q8CIE6
C	1229	PHE	-	expression tag	UNP Q8CIE6
C	1230	GLN	-	expression tag	UNP Q8CIE6
C	1231	GLY	-	expression tag	UNP Q8CIE6
C	1232	PRO	-	expression tag	UNP Q8CIE6
C	1233	SER	-	expression tag	UNP Q8CIE6
C	1234	ALA	-	expression tag	UNP Q8CIE6
C	1235	TRP	-	expression tag	UNP Q8CIE6
C	1236	SER	-	expression tag	UNP Q8CIE6
C	1237	HIS	-	expression tag	UNP Q8CIE6
C	1238	PRO	-	expression tag	UNP Q8CIE6
C	1239	GLN	-	expression tag	UNP Q8CIE6
C	1240	PHE	-	expression tag	UNP Q8CIE6
C	1241	GLU	-	expression tag	UNP Q8CIE6
C	1242	LYS	-	expression tag	UNP Q8CIE6
C	1243	GLY	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	GLY	-	expression tag	UNP Q8CIE6
C	1245	GLY	-	expression tag	UNP Q8CIE6
C	1246	SER	-	expression tag	UNP Q8CIE6
C	1247	GLY	-	expression tag	UNP Q8CIE6
C	1248	GLY	-	expression tag	UNP Q8CIE6
C	1249	GLY	-	expression tag	UNP Q8CIE6
C	1250	SER	-	expression tag	UNP Q8CIE6
C	1251	GLY	-	expression tag	UNP Q8CIE6
C	1252	GLY	-	expression tag	UNP Q8CIE6
C	1253	SER	-	expression tag	UNP Q8CIE6
C	1254	ALA	-	expression tag	UNP Q8CIE6
C	1255	TRP	-	expression tag	UNP Q8CIE6
C	1256	SER	-	expression tag	UNP Q8CIE6
C	1257	HIS	-	expression tag	UNP Q8CIE6
C	1258	PRO	-	expression tag	UNP Q8CIE6
C	1259	GLN	-	expression tag	UNP Q8CIE6
C	1260	PHE	-	expression tag	UNP Q8CIE6
C	1261	GLU	-	expression tag	UNP Q8CIE6
C	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 3 is a protein called COATOMER SUBUNIT BETA'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	803	Total	C	N	O	0	0
			3211	1606	803	802		

- Molecule 4 is a protein called COATOMER SUBUNIT GAMMA-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	550	Total	C	N	O	0	0
			2199	1100	550	549		

- Molecule 5 is a protein called COATOMER SUBUNIT ZETA-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	139	Total	C	N	O	0	0
			555	278	139	138		

- Molecule 6 is a protein called COATOMER SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	813	Total	C	N	O	0	0
			3250	1626	813	811		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	MET	-	expression tag	UNP Q9JIF7
G	-13	HIS	-	expression tag	UNP Q9JIF7
G	-12	HIS	-	expression tag	UNP Q9JIF7
G	-11	HIS	-	expression tag	UNP Q9JIF7
G	-10	HIS	-	expression tag	UNP Q9JIF7
G	-9	HIS	-	expression tag	UNP Q9JIF7
G	-8	HIS	-	expression tag	UNP Q9JIF7
G	-7	GLU	-	expression tag	UNP Q9JIF7
G	-6	ASN	-	expression tag	UNP Q9JIF7
G	-5	LEU	-	expression tag	UNP Q9JIF7
G	-4	TYR	-	expression tag	UNP Q9JIF7
G	-3	PHE	-	expression tag	UNP Q9JIF7
G	-2	GLN	-	expression tag	UNP Q9JIF7
G	-1	GLY	-	expression tag	UNP Q9JIF7
G	0	HIS	-	expression tag	UNP Q9JIF7


- Molecule 7 is a protein called COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	380	Total	C	N	O	0	0
			1520	760	380	380		



• Molecule 1: ADP-RIBOSYLATION FACTOR 1

MET	GLY	LEU	PHE	ALA	SER	LYS	LEU	PHE	SER	ASN	LEU	PHE	GLY	ASN	LYS	GLU	M18	S176	LEU	LYS	ASN	SER	THR
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Chain B:  88% 12%

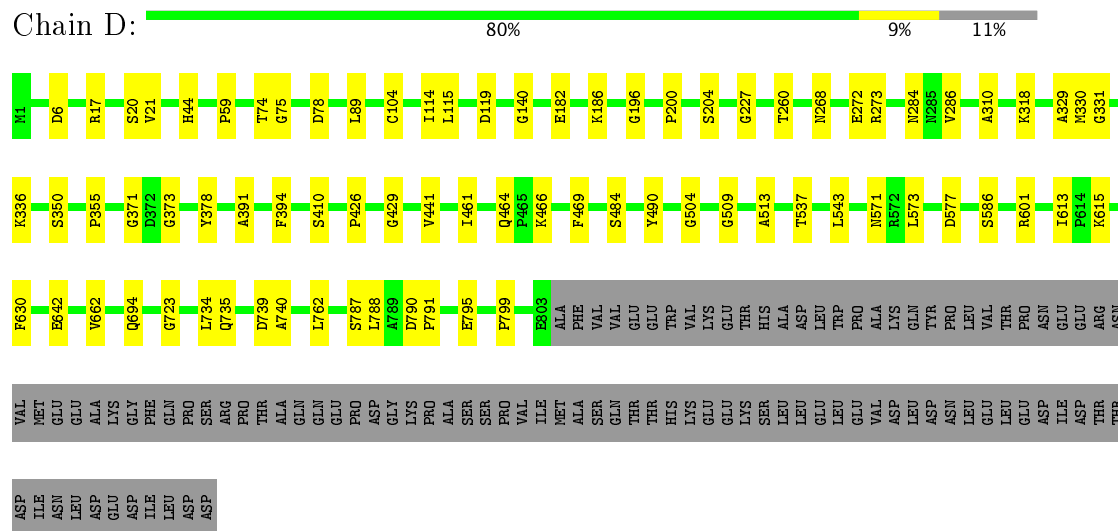
MET	GLY	LEU	PHE	ALA	SER	LYS	LEU	PHE	SER	ASN	LEU	PHE	GLY	ASN	LYS	GLU	M18	S176	LEU	LYS	ASN	SER	THR
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Chain C: 

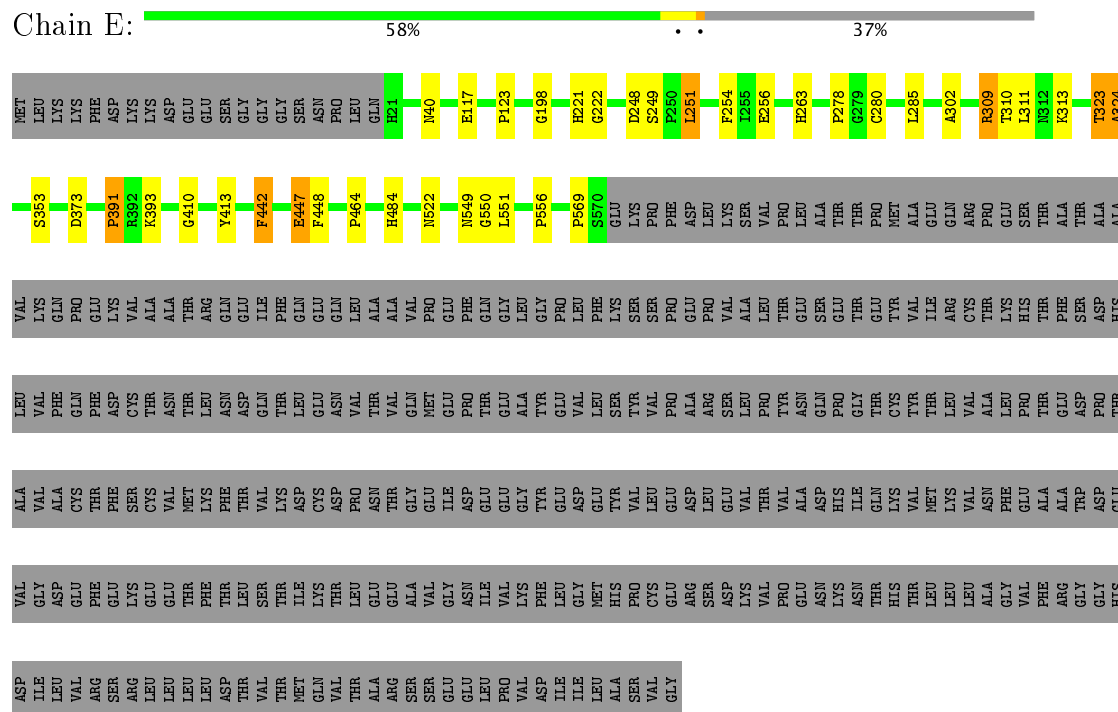
ASN	ALA	ALA	ALA	HIS	LEU	A799	M424	MI
ASN	GLN	GLN	GLY	ILE	GLY	TR812	R425	R11
PHE	LEU	LEU	LYS	ALA	GLY	TR813	K441	L15
PHE	ILE	THR	GLY	SER	GLU	LYS	N442	V64
LYS	ILE	THR	VAL	PHE	GLU	GLY	M452	Q63
ASN	CYS	CYS	PRO	GLU	GLY	PHE	A469	Y105
PHE	ARG	ALA	ALA	THR	GLY	PHE	D470	Y130
LYS	GLU	VAL	VAL	ALA	GLY	GLU	I488	G133
THR	TYR	GLY	GLY	MET	TRP	GLY	A498	Y137
ALA	ILE	THR	LEU	ARG	ASP	GLY	A498	R168
ALA	VAL	VAL	LYS	LEU	VAL	ILE	A498	G186
ALA	GLY	THR	LEU	HIS	GLU	GLY	E526	T193
PHE	GLY	ASN	ASP	HIS	GLU	SER	E526	V200
ALA	CYS	ASP	ASP	ASP	ASP	LYS	I488	E204
ARG	MET	LEU	LEU	GLN	LEU	GLY	S538	D205
ARG	GLU	ILE	ILE	VAL	GLU	LYS	S538	G223
ILE	ILE	GLN	GLN	GLY	GLU	LYS	S546	D226
LEU	ILE	ARG	ARG	VAL	PRO	GLY	S546	R227
LEU	ARG	LEU	LEU	ILE	PRO	ALA	G559	G247
GLY	LYS	GLN	GLN	GLN	GLU	LEU	G559	K271
PRO	LYS	LEU	CYS	PHE	LEU	ALA	R572	S272
LYS	PRO	TYR	TYR	PRO	ASP	ALA	R572	I273
LYS	GLN	LYS	GLN	GLY	VAL	VAL	P594	F317
PRO	GLU	GLU	LEU	TYR	SER	ALA	P594	K337
THR	THR	THR	THR	GLN	GLY	THR	K619	D345
VAL	THR	THR	THR	LEU	VAL	GLY	K619	S348
ASP	ASP	VAL	VAL	PHE	SER	ASP	V631	S349
GLN	GLN	LYS	LYS	LEU	SER	VAL	I670	A353
THR	LYS	PHE	PHE	GLN	GLY	THR	V631	C380
ARG	ARG	GLY	GLY	THR	GLY	GLY	S624	E387
ILE	ILE	GLY	THR	TYR	ALA	THR	A627	P790
LEU	ILE	GLY	GLY	TYR	GLU	GLY	A627	A400
SER	CYS	ALA	ALA	ARG	ASP	GLY	Q630	K793
LEU	GLY	VAL	VAL	GLY	PHE	TRP	K631	R422
ALA	MET	GLU	GLU	ARG	PHE	GLY	K631	
ALA	ALA	LYS	LYS	THR	VAL	ASP	V642	
GLU	ALA	PHE	ALA	THR	PRO	ALA	V642	
LYS	TYR	ARG	TYR	TYR	PRO	GLY	Q684	
ASN	PHE	SER	GLN	TYR	THR	LEU	G685	
PRO	THR	THR	ILE	ALA	LYS	GLN	N686	
THR	HIS	SER	LEU	LEU	GLY	LEU	N686	
ASP	SER	LEU	PRO	PRO	THR	ASP	K698	
ALA	ASN	SER	LEU	CYS	SER	GLY	K698	
CYS	VAL	VAL	VAL	LEU	PRO	ASP	I709	
GLN	PRO	PRO	PRO	PRO	THR	GLY	I709	
PRO	PRO	LEU	SER	SER	GLN	PHE	G731	
VAL	VAL	LEU	LEU	ILE	ILE	VAL	H732	
HIS	HIS	VAL	VAL	TYR	TRP	GLY	G740	
ASN	MET	VAL	VAL	TYR	CYS	ALA	G740	
MET	ILE	ASP	ASP	TYR	ASN	PRO	P780	
HIS	LEU	ASN	ASN	PRO	ASN	GLY	E781	
ASN	VAL	LYS	LYS	PRO	SER	GLY	P780	
PRO	LEU	GLN	GLN	ARG	GLN	LEU	E781	
PHE	ARG	THR	GLU	ASN	LEU	GLY	P790	
ASP	THR	ILE	ILE	TRP	PRO	GLY	A400	
ILE	LEU	ALA	GLY	LYS	VAL	ASP	K793	
LEU	LEU	THR	THR	ASP	GLN	VAL	R422	

[illegible]

• Molecule 3: COATOMER SUBUNIT BETA'



- Molecule 4: COATOMER SUBUNIT GAMMA-1



• Molecule 5: COATOMER SUBUNIT ZETA-1







## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of tilted images used	2122	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	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	0.43	0/635	0.69	0/792
1	B	0.43	0/635	0.69	0/792
2	C	1.55	8/3250 (0.2%)	1.71	14/4061 (0.3%)
3	D	1.60	17/3210 (0.5%)	1.72	23/4011 (0.6%)
4	E	1.52	2/2198 (0.1%)	1.58	9/2746 (0.3%)
5	F	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
6	G	1.50	7/3248 (0.2%)	1.71	22/4057 (0.5%)
7	H	1.21	0/1518	1.34	8/1893 (0.4%)
All	All	1.45	35/15248 (0.2%)	1.60	79/19043 (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
2	C	0	4
3	D	0	2
4	E	0	4
5	F	0	1
6	G	0	14
All	All	0	25

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	621	VAL	C-N	6.92	1.45	1.33
3	D	330	MET	N-CA	-6.75	1.32	1.46
4	E	198	GLY	CA-C	-6.44	1.41	1.51
3	D	378	TYR	N-CA	-6.39	1.33	1.46
3	D	537	THR	N-CA	-6.33	1.33	1.46

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	496	GLU	N-CA-C	7.82	132.10	111.00
4	E	302	ALA	C-N-CA	7.06	139.35	121.70
2	C	54	VAL	N-CA-C	-6.92	92.31	111.00
6	G	486	ILE	O-C-N	-6.81	108.17	121.10
6	G	869	THR	N-CA-C	-6.73	92.83	111.00

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	317	PHE	Mainchain
2	C	380	CYS	Mainchain
2	C	559	GLY	Mainchain
2	C	63	GLN	Peptide
3	D	44	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	636	0	181	0	0
1	B	636	0	181	0	0
2	C	3251	0	869	0	0
3	D	3211	0	880	0	0
4	E	2199	0	570	1	0
5	F	555	0	148	0	0
6	G	3250	0	833	0	0
7	H	1520	0	406	4	0
All	All	15258	0	4068	5	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 0.

All (5) 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)
7:H:296:GLU:CA	7:H:368:THR:H	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:356:ASN:CA	7:H:362:LEU:H	2.10	0.65
7:H:356:ASN:C	7:H:362:LEU:H	2.20	0.45
4:E:249:SER:C	4:E:251:LEU:H	2.23	0.41
7:H:356:ASN:CA	7:H:362:LEU:N	2.83	0.41

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	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
1	B	157/181 (87%)	153 (98%)	4 (2%)	0	100	100
2	C	811/1262 (64%)	671 (83%)	97 (12%)	43 (5%)	2	26
3	D	801/905 (88%)	700 (87%)	64 (8%)	37 (5%)	3	28
4	E	548/874 (63%)	492 (90%)	27 (5%)	29 (5%)	2	26
5	F	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	12	53
6	G	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1	16
7	H	376/511 (74%)	336 (89%)	31 (8%)	9 (2%)	7	42
All	All	3796/5059 (75%)	3291 (87%)	318 (8%)	187 (5%)	5	27

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	11	ARG
2	C	227	ARG
2	C	526	GLU
2	C	572	ARG
2	C	686	ASN

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.