



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4BOI  
EMDB ID: : EMD-2377  
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes class A  
Authors : Zuber, B.; Unwin, N.  
Deposited on : 2013-05-20  
Resolution : 41.00 Å(reported)  
Based on PDB ID : 2BG9

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](mailto: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

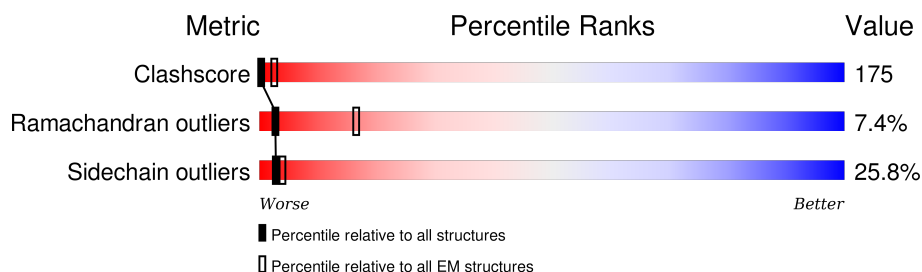
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 41.00 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  $\geq 3$ , 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	461	
1	D	461	
2	B	493	
3	C	522	
4	E	505	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14924 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
1	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

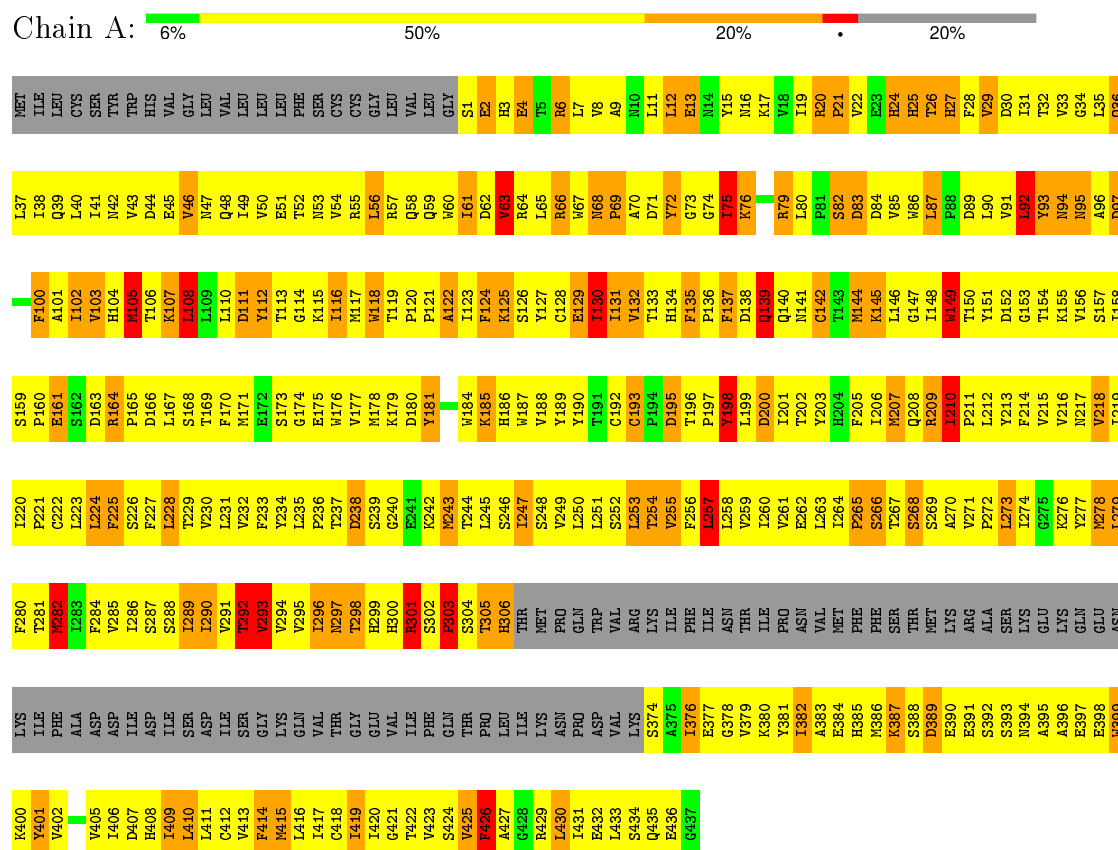
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

### 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: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA





M465	ASN	GLU	V285	R223	M160	G100	S40
V466	ASN	ILE	P286	K224	D161	Q101	M41
L467	GLU	GLU	L287	P225	L162	Y102	L42
G468	ASN	GLN	I288	L226	MET	N103	I43
T469	ILE	PRO	G289	F227	THR	M104	T43
I470	ALA	ASP	K290	Y228	ASP	A105	S44
F471	ALA	TRP	Y291	Y229	THR	Y106	L45
L472	SER	GLN	L292	L230	ILE	F107	K46
F473	ASP	ASN	M293	F231	ASP	C108	T48
V474	GLN	ASP	F294	P232	GLY	M109	D49
M475	LEU	LEU	L295	L233	LYS	V110	E50
G476	HIS	LYS	M296	T234	ASP	L111	T51
M477	ASP	LEU	S297	P235	TYR	V112	L52
F478	ILE	ARG	L298	L238	ILE	R113	T53
M479	GLU	ARG	V299	M299	ILE	P114	T54
R480	LYS	SER	S300	V239	GLU	M115	N55
P481	G421	SER	G301	L239	TRP	G116	V56
P482	G422	SER	V302	F241	ILE	Y117	M57
A483	I423	VAL	V303	L242	I178	V118	M58
K484	D424	GLY	V304	A243	I179	T119	D59
P485	S425	TYR	N305	A244	D180	W120	H60
PHE	T426	ILE	C306	L245	P181	L121	A61
GLU	N427	SER	G307	A246	E182	P122	W62
GLY	Y428	LYS	I308	F247	A183	P123	Y63
ASP	I429	ALA	V309	Y248	F184	P124	R63
PRO	V430	GLN	L310	L249	T185	A124	D64
PHE	K431	GLU	N311	P250	E186	F126	H65
ASP	Q432	TYR	F312	A251	N187	G127	L67
TYR	L433	PHE	H313	E252	G188	S128	T68
SER	K434	ASN	F314	S253	E189	S129	M69
SER	E435	ILE	R315	K256	W190	C130	N70
ASP	K436	LYS	T316	M257	E191	P131	A71
HIS	N437	SER	P317	S258	I192	I132	S72
PRO	A438	ARG	S318	T259	I193	N133	E73
ARG	Y439	SER	T319	T259	H194	V134	Y74
CYS	D440	GLU	H320	A260	K195	L135	S75
ALA	E441	LEU	VAL	L261	K198	Y136	D76
	E442	MET	SER	C262	K199	F137	I77
	V443	PHE	SER	V263	L198	P138	S78
	G444	GLU	THR	L264	N200	F139	I79
	M445	LYS	ARG	L265	T201	D140	L80
	M446	GLN	VAL	A266	Y202	W441	R81
	M447	SER	LYS	Q267	G203	Q142	L82
	L448	GLU	GLN	A268	D204	N143	R83
	V449	ARG	ILE	V269	K205	C144	P84
	G450	HIS	PHE	F270	F206	S145	E85
	Q451	GLY	LEU	L271	P207	L146	L86
	T452	LEU	GLU	L272		K147	I87
	I453	VAL	LYS	L273	N211	F148	M88
	D454	PRO	LEU	T274	Y212	T149	I89
	R455	ARG	PRO	S275	Q213	A150	P90
	L456	VAL	ARG	Q276	D214	L151	D91
	S457	THR	ILE	R277	V215	N152	I92
	M458	PRO	LEU	L278	T216	Y153	V93
	F459	ARG	HIS	P279	T217	N154	L94
	I460	ILE	MET	E280	G218	A155	Q95
	T461	GLY	SER	T281	L219	N156	N96
	Y462	PHE	ARG	A282	T220	E157	N97
	P463	GLY	VAL	L283	T221	I158	N98
	V464	ASN	ASP	E284	R222	S159	D99

• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E: 6% 46% 18% • 27%

ASP	LEU	ALA	ASN	PHE	ALA	PRO	GLU	ARG	GLU	LYS	SER	PHE	GLY	ILE	MET	ILE	ALA	GLU	VAL	ARG	SER	N1	E2	E3	G4	R5	L6	I7	E8	K9	L10	L11	G12	L13	D13	Y14	D15	K16	V17	R17	I18	K19	P20	A21	K22	T23	L24	D25	H26	V27	I28	D29	V30	T31	L32	K33	L34	T35	L36	T37	N38	L39	I40	S41	L42	M43
E44	K45	E46	E47	A48	L49	T50	T51	N52	V53	W54	I55	E56	I57	Q58	W59	N60	D61	Y62	R63	L64	W65	N66	N67	T68	S69	E70	E71	E72	G73	I74	D75	L76	V77	R78	I79	P80	S81	E82	L83	L84	W85	L86	P87	D88	W89	V90	L91	E92	N93	N94	Y95	D96	G97	Q98	F99	E100	I101	A102	Y103							
Y104	A105	M106	V107	L108	V109	Y110	M111	D112	G113	S114	M115	V116	W117	L118	P119	A120	A121	I122	Y123	L124	S125	T126	C127	P128	I129	A130	V131	T132	Y133	F134	P135	F136	D137	M138	Q139	N140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	N150	N151	A152	H153	E154	V155	N156	L157	Q158	L159	S160	A161	E162	E163							
G164	GLU	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	N180	G181	E182	W183	I184	I185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	H195	V196	Q197	L198	L199	K200	D201	D202	L203	D204	F205	Q206	E207	L208	I209	F210	F211	L212	T213	T214	Q215	R216	S217	L218	P219	F220	Y221	T222	T223							
N224	I225	A226	A227	P228	C229	V230	L231	I232	S233	S234	L235	V236	V237	L238	V239	Y240	F241	L242	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	T252	L253	S254	L255	S256	V257	L258	L259	A260	Q261	T262	L263	F264	L265	P266	L267	I268	A269	Q270	K271	L272	P273	E274	T275	S276	L277	N278	V279	P280	L281	L282	G283							
K284	T285	L286	T287	F288	V289	W290	F291	V292	S293	L294	V295	L296	V297	T298	N299	C300	V301	I302	V303	L304	N305	V306	S307	L308	R309	T310	D311	N312	M313	L314	SER	LEU	SER	GLN	GLU	LYS	ILE	LYS	HIS	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464								
GLU	LYS	PRO	GLN	PRO	ARG	ARG	ARG	ILE	SER	PHE	GLY	ILE	MET	ILE	ILE	ALA	GLU	GLU	TYR	TYR	LEU	LYS	LYS	PRO	ARG	SER	GLU	GLU	LEU	PHE	GLU	GLN	LYS	ASP	ILE	LYS	HIS	GLY	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464									
ASP	LEU	ALA	ASN	PHE	ALA	PRO	GLU	ARG	GLU	LYS	SER	PHE	GLY	ILE	MET	ILE	ALA	GLU	VAL	ARG	SER	N1	E2	E3	G4	R5	L6	I7	E8	K9	L10	L11	G12	L13	D13	Y14	D15	K16	V17	R17	I18	K19	P20	A21	K22	T23	L24	D25	H26	V27	I28	D29	V30	T31	L32	K33	L34	T35	L36	T37	N38	L39	I40	S41	L42	M43
E44	K45	E46	E47	A48	L49	T50	T51	N52	V53	W54	I55	E56	I57	Q58	W59	N60	D61	Y62	R63	L64	W65	N66	N67	T68	S69	E70	E71	E72	G73	I74	D75	L76	V77	R78	I79	P80	S81	E82	L83	L84	W85	L86	P87	D88	W89	V90	L91	E92	N93	N94	Y95	D96	G97	Q98	F99	E100	I101	A102	Y103							
Y104	A105	M106	V107	L108	V109	Y110	M111	D112	G113	S114	M115	V116	W117	L118	P119	A120	A121	I122	Y123	L124	S125	T126	C127	P128	I129	A130	V131	T132	Y133	F134	P135	F136	D137	M138	Q139	N140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	N150	N151	A152	H153	E154	V155	N156	L157	Q158	L159	S160	A161	E162	E163							
G164	GLU	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	N180	G181	E182	W183	I184	I185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	H195	V196	Q197	L198	L199	K200	D201	D202	L203	D204	F205	Q206	E207	L208	I209	F210	F211	L212	T213	T214	Q215	R216	S217	L218	P219	F220	Y221	T222	T223							
N224	I225	A226	A227	P228	C229	V230	L231	I232	S233	S234	L235	V236	V237	L238	V239	Y240	F241	L242	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	T252	L253	S254	L255	S256	V257	L258	L259	A260	Q261	T262	L263	F264	L265	P266	L267	I268	A269	Q270	K271	L272	P273	E274	T275	S276	L277	N278	V279	P280	L281	L282	G283							
K284	T285	L286	T287	F288	V289	W290	F291	V292	S293	L294	V295	L296	V297	T298	N299	C300	V301	I302	V303	L304	N305	V306	S307	L308	R309	T310	D311	N312	M313	L314	SER	LEU	SER	GLN	GLU	LYS	ILE	LYS	HIS	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464								
GLU	LYS	PRO	GLN	PRO	ARG	ARG	ARG	ILE	SER	PHE	GLY	ILE	MET	ILE	ILE	ALA	GLU	GLU	TYR	TYR	LEU	LYS	LYS	PRO	ARG	SER	GLU	GLU	LEU	PHE	GLU	GLN	LYS	ASP	ILE	LYS	HIS	GLY	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464									
ASP	LEU	ALA	ASN	PHE	ALA	PRO	GLU	ARG	GLU	LYS	SER	PHE	GLY	ILE	MET	ILE	ALA	GLU	VAL	ARG	SER	N1	E2	E3	G4	R5	L6	I7	E8	K9	L10	L11	G12	L13	D13	Y14	D15	K16	V17	R17	I18	K19	P20	A21	K22	T23	L24	D25	H26	V27	I28	D29	V30	T31	L32	K33	L34	T35	L36	T37	N38	L39	I40	S41	L42	M43
E44	K45	E46	E47	A48	L49	T50	T51	N52	V53	W54	I55	E56	I57	Q58	W59	N60	D61	Y62	R63	L64	W65	N66	N67	T68	S69	E70	E71	E72	G73	I74	D75	L76	V77	R78	I79	P80	S81	E82	L83	L84	W85	L86	P87	D88	W89	V90	L91	E92	N93	N94	Y95	D96	G97	Q98	F99	E100	I101	A102	Y103							
Y104	A105	M106	V107	L108	V109	Y110	M111	D112	G113	S114	M115	V116	W117	L118	P119	A120	A121	I122	Y123	L124	S125	T126	C127	P128	I129	A130	V131	T132	Y133	F134	P135	F136	D137	M138	Q139	N140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	N150	N151	A152	H153	E154	V155	N156	L157	Q158	L159	S160	A161	E162	E163							
G164	GLU	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	N180	G181	E182	W183	I184	I185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	H195	V196	Q197	L198	L199	K200	D201	D202	L203	D204	F205	Q206	E207	L208	I209	F210	F211	L212	T213	T214	Q215	R216	S217	L218	P219	F220	Y221	T222	T223							
N224	I225	A226	A227	P228	C229	V230	L231	I232	S233	S234	L235	V236	V237	L238	V239	Y240	F241	L242	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	T252	L253	S254	L255	S256	V257	L258	L259	A260	Q261	T262	L263	F264	L265	P266	L267	I268	A269	Q270	K271	L272	P273	E274	T275	S276	L277	N278	V279	P280	L281	L282	G283							
K284	T285	L286	T287	F288	V289	W290	F291	V292	S293	L294	V295	L296	V297	T298	N299	C300	V301	I302	V303	L304	N305	V306	S307	L308	R309	T310	D311	N312	M313	L314	SER	LEU	SER	GLN	GLU	LYS	ILE	LYS	HIS	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464								
GLU	LYS	PRO	GLN	PRO	ARG	ARG	ARG	ILE	SER	PHE	GLY	ILE	MET	ILE	ILE	ALA	GLU	GLU	TYR	TYR	LEU	LYS	LYS	PRO	ARG	SER	GLU	GLU	LEU	PHE	GLU	GLN	LYS	ASP	ILE	LYS	HIS	GLY	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464									
ASP	LEU	ALA	ASN	PHE	ALA	PRO	GLU	ARG	GLU	LYS	SER	PHE	GLY	ILE	MET	ILE	ALA	GLU	VAL	ARG	SER	N1	E2	E3	G4	R5	L6	I7	E8	K9	L10	L11	G12	L13	D13	Y14	D15	K16	V17	R17	I18	K19	P20	A21	K22	T23	L24	D25	H26	V27	I28	D29	V30	T31	L32	K33	L34	T35	L36	T37	N38	L39	I40	S41	L42	M43
E44	K45	E46	E47	A48	L49	T50	T51	N52	V53	W54	I55	E56	I57	Q58	W59	N60	D61	Y62	R63	L64	W65	N66	N67	T68	S69	E70	E71	E72	G73	I74	D75	L76	V77	R78	I79	P80	S81	E82	L83	L84	W85	L86	P87	D88	W89	V90	L91	E92	N93	N94	Y95	D96	G97	Q98	F99	E100	I101	A102	Y103							
Y104	A105	M106	V107	L108	V109	Y110	M111	D112	G113	S114	M115	V116	W117	L118	P119	A120	A121	I122	Y123	L124	S125	T126	C127	P128	I129	A130	V131	T132	Y133	F134	P135	F136	D137	M138	Q139	N140	C141	S142	L143	V144	F145	R146	S147	Q148	T149	N150	N151	A152	H153	E154	V155	N156	L157	Q158	L159	S160	A161	E162	E163							
G164	GLU	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	N180	G181	E182	W183	I184	I185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	H195	V196	Q197	L198	L199	K200	D201	D202	L203	D204	F205	Q206	E207	L208	I209	F210	F211	L212	T213	T214	Q215	R216	S217	L218	P219	F220	Y221	T222	T223							
N224	I225	A226	A227	P228	C229	V230	L231	I232	S233	S234	L235	V236	V237	L238	V239	Y240	F241	L242	P243	A244	Q245	A246	G247	G248	Q249	K250	C251	T252	L253	S254	L255	S256	V257	L258	L259	A260	Q261	T262	L263	F264	L265	P266	L267	I268	A269	Q270	K271	L272	P273	E274	T275	S276	L277	N278	V279	P280	L281	L282	G283							
K284	T285	L286	T287	F288	V289	W290	F291	V292	S293	L294	V295	L296	V297	T298	N299	C300	V301	I302	V303	L304	N305	V306	S307	L308	R309	T310	D311	N312	M313	L314	SER	LEU	SER	GLN	GLU	LYS	ILE	LYS	HIS	LEU	PHE	LEU	ASN	LYS	MET	PRO	THR	GLY	ASP	ASP	GLY	THR	THR	VAL	ASP	T462	L463	A464								
GLU	LYS	PRO	GLN	PRO	ARG	ARG	ARG	ILE	SER	PHE	GLY	ILE	MET	ILE	ILE</																																																			

I465	F466	G469	H470	L471	I472	Q473	V474	P475	E476	F477	PRO	PHE	PRO	PRO	GLY	ASP	PRO	ARG	LYS	TYR	VAL	PRO
------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided, Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	69000	Depositor
Image detector	GATAN US4000	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	3/3069 (0.1%)	1.03	10/4186 (0.2%)
1	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
2	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
3	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
4	E	0.74	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20883 (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	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-8.42	1.14	1.34
1	A	118	TRP	CB-CG	7.88	1.64	1.50
1	D	208	GLN	C-N	7.58	1.51	1.34
4	E	8	GLU	CB-CG	6.57	1.64	1.52
3	C	265	LEU	C-N	6.20	1.48	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	ALA	N-CA-CB	10.39	124.65	110.10
4	E	198	LEU	CA-CB-CG	7.21	131.89	115.30
3	C	315	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	A	209	ARG	NE-CZ-NH2	7.12	123.86	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.67	96.74	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	63	TYR	Sidechain
3	C	74	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	72	TYR	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	A	2991	0	3005	1079	0
1	D	2991	0	3006	1058	0
2	B	2972	0	2952	1094	0
3	C	2983	0	2987	1161	0
4	E	2987	0	2994	1085	0
All	All	14924	0	14944	5215	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 175.

The worst 5 of 5215 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)
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.51
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.49
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.45
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.44
3:C:316:THR:CG2	3:C:317:PRO:HD2	1.53	1.38

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	366/461 (79%)	288 (79%)	50 (14%)	28 (8%)	1	20
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
2	B	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	1	17
3	C	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	3	31
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1	22
All	All	1825/2442 (75%)	1425 (78%)	265 (14%)	135 (7%)	3	21

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	27	HIS
1	A	76	LYS
1	A	83	ASP
1	A	102	ILE

### 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	A	343/427 (80%)	248 (72%)	95 (28%)	0	4
1	D	343/427 (80%)	258 (75%)	85 (25%)	1	6
2	B	340/449 (76%)	262 (77%)	78 (23%)	1	7
3	C	335/475 (70%)	243 (72%)	92 (28%)	0	4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	337/463 (73%)	249 (74%)	88 (26%)	0 5
All	All	1698/2241 (76%)	1260 (74%)	438 (26%)	3 5

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	106	TYR
3	C	315	ARG
4	E	217	LYS
3	C	130	CYS
3	C	241	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
1	D	42	ASN
4	E	197	GLN
3	C	231	ASN
3	C	479	ASN

### 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.