



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4BOR
EMDB ID: : EMD-2382
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes class D
Authors : Zuber, B.; Unwin, N.
Deposited on : 2013-05-22
Resolution : 42.00 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
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

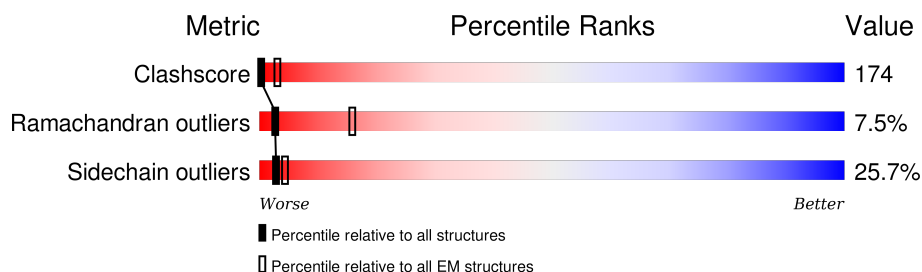
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 42.00 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	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		

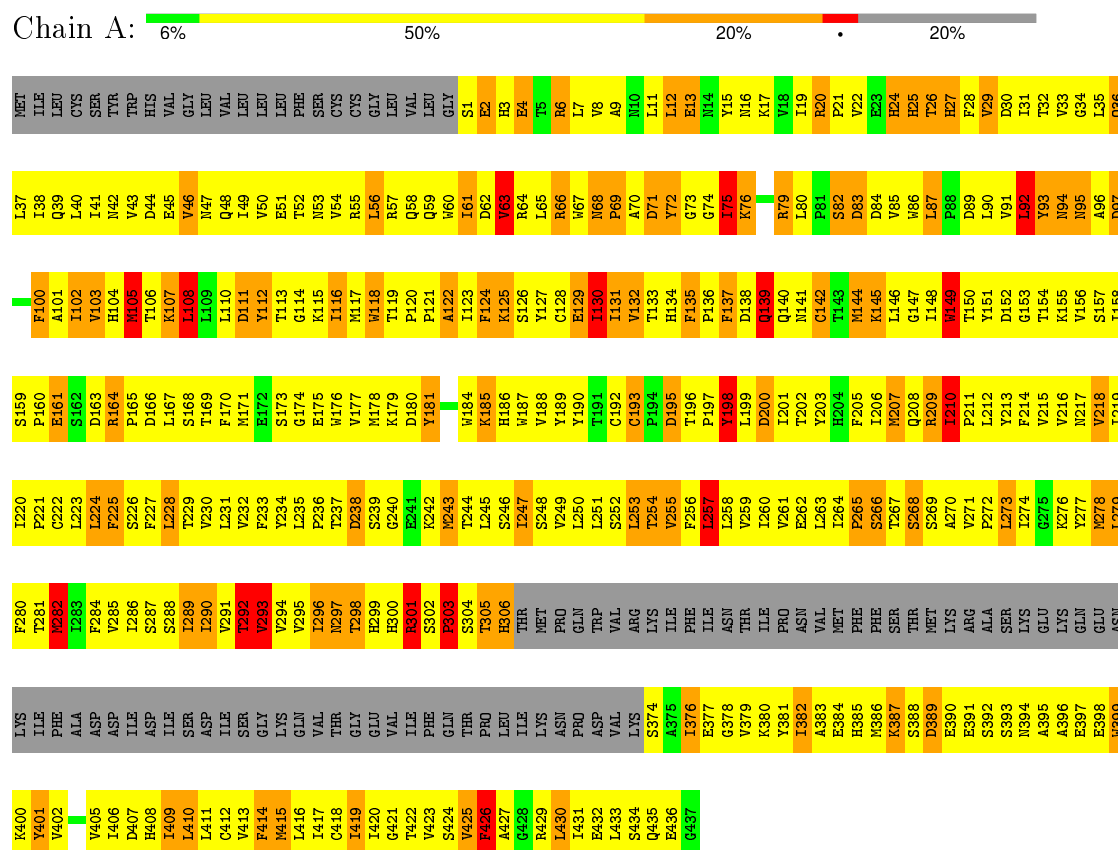
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

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

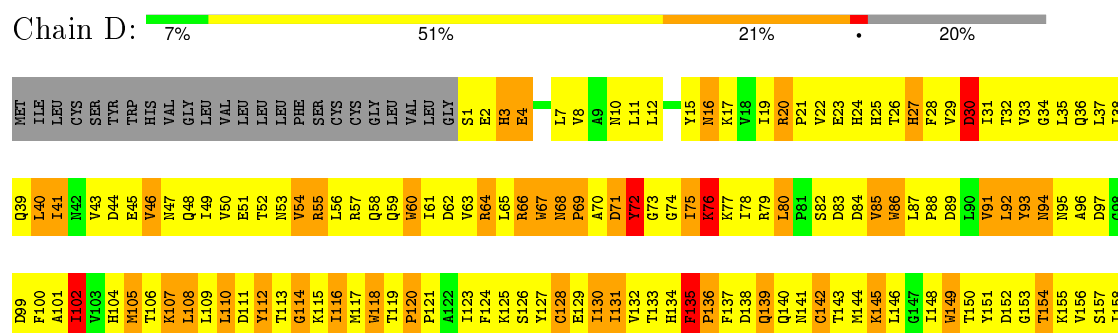
3 Residue-property plots

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



• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA






S40	M41	I43	I43	S44	K46	E47	T48	D49	E50	T51	L52	T53	T54	N55	V56	W57	M58	H60	A61	W62	Y63	D64	H65	R66	L67	T68	W69	N70	A71	S72	E73	Y74	S75	D76	I77	S78	I79	R80	R81	L82	R83	P84	E85	L86	I87	W88	I89	D90	I92	V93	L94	Q95	N96	N97	N98	D99					
G100	Q101	Y102	M103	V104	A105	F107	C108	M109	Y110	L111	V112	R113	P114	M115	G116	Y117	V118	T119	W120	L121	P122	P123	A124	F125	F126	R127	S128	S129	C130	P131	I132	N133	V134	L135	F136	F137	P138	F139	D140	W141	Q142	N143	C144	S145	L146	K147	F148	T149	A150	L151	Y152	Y153	L154	A155	N156	E157	I158	S159			
M160	D161	L162	MET	THR	ASP	THR	ILE	ASP	GLY	LYS	ASP	TYR	PRO	GLU	TRP	ILE	I178	I179	D180	E181	E182	A183	F184	T185	E186	G188	E189	W190	I191	I192	I193	H194	K195	K198	K199	N200	I201	Y202	G203	K204	K205	F206	P207	N211	Y212	Q213	D214	T215	T216	F217	Y218	L219	I220	I221	R222						
R223	K224	L225	L226	F227	Y228	V229	M230	M231	F232	L233	T234	P235	L238	V239	M239	F234	L235	G301	V302	F303	V304	N305	C306	G307	I308	L310	N311	F312	H313	F314	R315	T316	M257	V263	L264	L265	A266	Q267	A268	V269	PHE	L271	L272	L273	L274	PRO	ARG	VAL	N152	R277	L278	PRO	HIS	MET	SER	ARG	VAL	ASP			
V285	P286	L287	L288	G289	K290	Y291	L292	M293	F294	L295	M296	S297	L298	V299	M299	G301	V302	F303	V304	N305	C306	G307	I308	L310	N311	F312	H313	F314	R315	T316	M257	V263	L264	L265	A266	Q267	A268	V269	PHE	L271	L272	L273	L274	PRO	ARG	VAL	N152	R277	L278	PRO	HIS	MET	SER	ARG	VAL	ASP					
GLU	ILE	GLN	GLN	PRO	ASP	TRP	GLN	ASN	ASP	LEU	LYS	LEU	ARG	ARG	ARG	SER	VAL	GLY	TYR	ILE	SER	LYS	ALA	GLN	GLU	GLU	TYR	PHE	ASN	ILE	LYS	SER	ARG	GLU	LEU	MET	PHE	GLU	THR	LYS	GLN	SER	GLU	ARG	VAL	THR	PRO	ARG	VAL	THR	ILE	GLY	PHE	GLY	ASN						
ASN	ASN	ASN	ASN	ILE	ALA	ALA	SER	ASP	GLN	LEU	HIS	ASP	GLU	LYS	LYS	G421	G422	I423	D424	S425	T426	N427	Y428	I429	V430	K431	Q432	T433	I434	K435	K436	N437	A438	Y439	D440	E441	E442	G443	G444	M445	M446	M447	L448	V449	G450	Q451	T452	I453	D454	R455	L456	S457	M458	F459	I460	I461	T462	P463	V464		
M465	V466	G468	T469	I470	F471	L472	F473	V474	M475	G476	M477	F478	M479	R480	P481	P482	A483	K484	P485	PHE	GLU	GLY	ASP	PRO	PHE	ASP	TYR	GLY	SER	SER	ASP	HIS	PRO	ARG	CYS	ALA	ALA	ALA	E442	G443	G444	M445	M446	M447	L448	V449	G450	Q451	T452	I453	D454	R455	L456	S457	M458	F459	I460	I461	T462	P463	V464

• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E: 6% 46% 18% • 27%

MET	VAL	LEU	THR	LEU	LEU	LEU	ILE	ILE	ILE	CYS	LEU	LEU	ALA	ALA	GLU	VAL	VAL	ARG	SER	N1	E2	G4	R5	L6	I7	E8	K9	L10	L11	G12	D13	Y14	D15	K16	R17	I18	K19	P20	A21	K22	T23	L24	D25	H26	V27	I28	D29	V30	T31	L32	K33	L34	T35	L36	T37	N38	F39	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	W66	W67	T68	S69	E70	Y71	A72	E73	E74	R75	L76	V77	W78	R79	P80	S81	E82	L83	L84	W85	L86	P87	D88	W89	Y90	L91	E92	N93	I94	Y95	D96	G97	Q98	F99	E100	I101	A102	Y103																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
Y104	A105	M106	V107	GLU	L108	V109	M110	D112	G113	S114	M115	V116	W117	L118	P119	M120	A121	I122	Y123	L124	S125	T126	C127	P128	I129	A130	V131	M132	E133	Y134	F135	F136	D137	M138	Q139	N140	C141	S142	L143	V144	F145	W146	S147	T148	T149	Y150	N151	A152	H153	E154	V155	N156	L157	Q158	L159	S160	A161	E162	E163																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G164	GLU	VAL	VAL	VAL	GLU	TRP	ILE	HIS	I172	D173	P174	E175	D176	F177	T178	E179	N180	G181	E182	W183	I184	L185	R186	H187	R188	P189	A190	K191	K192	N193	Y194	H195	V196	Q197	L198	L199	K200	D201	D202	L203	D204	F205	Q206	Q207	E208	T209	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	L252	T253	L254	S255	S256	V257	L258	L259	A260	Q261	T262	L263	F264	L265	L266	L267	I268	A269	Q270	K271	F272	P273	E274	S275	S276	L277	N278	V279	P280	L281	L282	G283																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
K284	T285	L286	T287	F288	V289	W290	F291	V292	S293	S294	V295	L296	V297	T298	N299	C300	V301	I302	V303	N304	L305	V306	S307	L308	R309	T310	D311	N312	N313	M314	L315	S316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067</

I465	F466	G469	H470	L471	I472	Q473	V474	P475	E476	F477	PRO	PHE	PRO	PRO	GLY	ASP	PRO	ARG	LYS	TYR	VAL	PRO
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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	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	0.73	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	-8.41	1.14	1.34
1	A	118	TRP	CB-CG	7.91	1.64	1.50
1	D	208	GLN	C-N	7.57	1.51	1.34
4	E	8	GLU	CB-CG	6.50	1.64	1.52
3	C	265	LEU	C-N	6.16	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	10.38	124.64	110.10
4	E	198	LEU	CA-CB-CG	7.19	131.83	115.30
3	C	315	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	209	ARG	NE-CZ-NH2	6.92	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.66	96.75	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	1073	0
1	D	2991	0	3006	1063	0
2	B	2972	0	2952	1078	0
3	C	2983	0	2987	1156	0
4	E	2987	0	2994	1087	0
All	All	14924	0	14944	5194	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 174.

The worst 5 of 5194 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	1.56
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	1.48
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	1.37

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%)	49 (13%)	29 (8%)	1	19
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	1	18
2	B	364/493 (74%)	273 (75%)	59 (16%)	32 (9%)	1	17
3	C	364/522 (70%)	289 (79%)	57 (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%)	264 (14%)	136 (8%)	3	21

5 of 136 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%)	244 (73%)	91 (27%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	337/463 (73%)	249 (74%)	88 (26%)	0	5
All	All	1698/2241 (76%)	1261 (74%)	437 (26%)	3	6

5 of 437 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	104	VAL
3	C	315	ARG
4	E	217	LYS
3	C	130	CYS
3	C	233	ILE

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 [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.