



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:36 AM GMT

PDB ID : 1DM5
Title : ANNEXIN XII E105K HOMOHEXAMER CRYSTAL STRUCTURE
Authors : Cartailier, J.P.; Haigler, H.T.; Luecke, H.
Deposited on : 1999-12-13
Resolution : 1.93 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

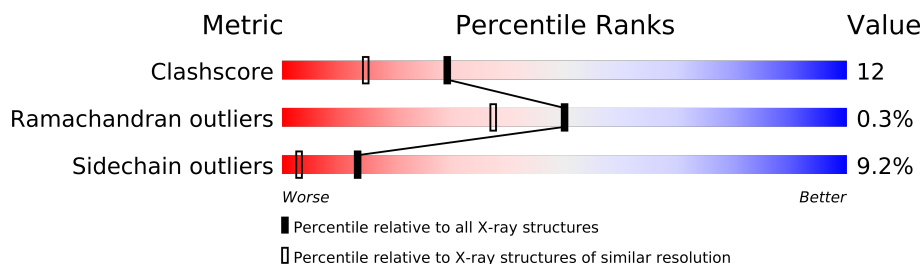
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.93 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	C	315	
1	D	315	
1	E	315	
1	F	315	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15709 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ANNEXIN XII E105K MUTANT HOMOHEXAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	B	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	C	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	D	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	E	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			
1	F	315	Total	C	N	O	S	0	0	0
			2462	1544	429	482	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	LYS	GLU	MUTATION	UNP P26256
B	105	LYS	GLU	MUTATION	UNP P26256
C	105	LYS	GLU	MUTATION	UNP P26256
D	105	LYS	GLU	MUTATION	UNP P26256
E	105	LYS	GLU	MUTATION	UNP P26256
F	105	LYS	GLU	MUTATION	UNP P26256

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Ca 2	0	0
2	A	2	Total 2	Ca 2	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total 140	O 140	0	0
3	B	193	Total 193	O 193	0	0
3	C	173	Total 173	O 173	0	0
3	D	152	Total 152	O 152	0	0
3	E	117	Total 117	O 117	0	0
3	F	151	Total 151	O 151	0	0

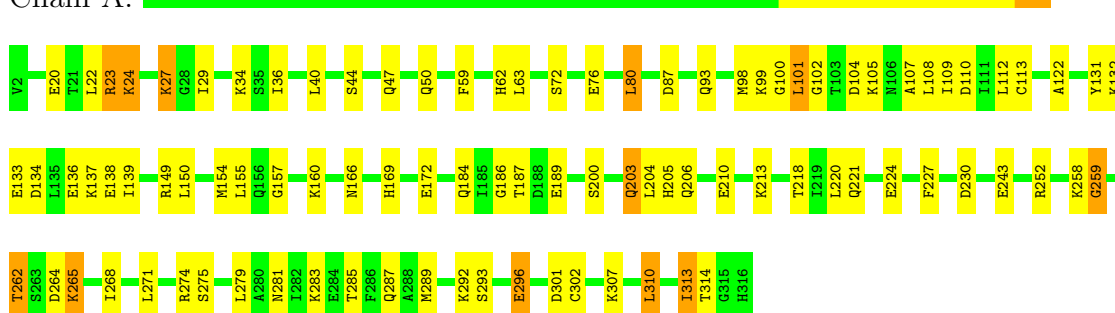
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain A:



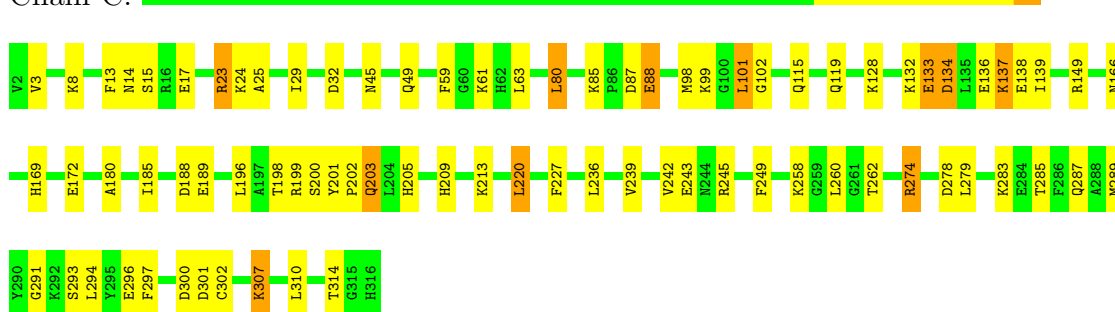
• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain B:



• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Chain C:



• Molecule 1: ANNEXIN XII E105K MUTANT HOMOHEXAMER

Q287	A288	M289	G290	Z291	K292	S293	L294	Y295	E296	F297	D300	D301	C302	K307	D308	L309	L310	L311	Q312	L313	T314	G315	H316	E142	K160	E161	D162	E163	P164	V165	N166	D173	Y178	Q179	I185	R189	S200	Y201	P202	Q203	L204	H205	S215	N216	L220	S228	G229	D230	L231	K232	V239	V242	E243	F249	K258	G259	L260	G261	T262	S263	D264	R274	D278	L279	K283	E284	T285	F286	E101	K102	G103	L104	Y105	Q106	L107	K108	L109	Y110	L111	K112	L113	Y114	L115	K116	L117	Y118	L119	K120	L121	Y122	L123	K124	L125	Y126	L127	K128	L129	Y130	L131	K132	L133	Y134	L135	K136	L137	Y138	L139	K140	L141	Y142	L143	K144	L145	Y146	L147	K148	L149	Y150	L151	K152	L153	Y154	L155	K156	L157	Y158	L159	K160	L161	Y162	L163	K164	L165	Y166	L167	K168	L169	Y170	L171	K172	L173	Y174	L175	K176	L177	Y178	L179	K180	L181	Y182	L183	K184	L185	Y186	L187	K188	L189	Y190	L191	K192	L193	Y194	L195	K196	L197	Y198	L199	K200	L201	Y202	L203	K204	L205	Y206	L207	K208	L209	Y210	L211	K212	L213	Y214	L215	K216	L217	Y218	L219	K220	L221	Y222	L223	K224	L225	Y226	L227	K228	L229	Y230	L231	K232	L233	Y234	L235	K236	L237	Y238	L239	K240	L241	Y242	L243	K244	L245	Y246	L247	K248	L249	Y250	L251	K252	L253	Y254	L255	K256	L257	Y258	L259	K260	L261	Y262	L263	K264	L265	Y266	L267	K268	L269	Y270	L271	K272	L273	Y274	L275	K276	L277	Y278	L279	K280	L281	Y282	L283	K284	L285	Y286	L287	K288	L289	Y290	L291	K292	L293	Y294	L295	K296	L297	Y298	L299	K300	L301	Y302	L303	K304	L305	Y306	L307	K308	L309	Y310	L311	K312	L313	Y314	L315	K316	L317	Y318	L319	K320	L321	Y322	L323	K324	L325	Y326	L327	K328	L329	Y330	L331	K332	L333	Y334	L335	K336	L337	Y338	L339	K340	L341	Y342	L343	K344	L345	Y346	L347	K348	L349	Y350	L351	K352	L353	Y354	L355	K356	L357	Y358	L359	K360	L361	Y362	L363	K364	L365	Y366	L367	K368	L369	Y370	L371	K372	L373	Y374	L375	K376	L377	Y378	L379	K380	L381	Y382	L383	K384	L385	Y386	L387	K388	L389	Y390	L391	K392	L393	Y394	L395	K396	L397	Y398	L399	K400	L401	Y402	L403	K404	L405	Y406	L407	K408	L409	Y410	L411	K412	L413	Y414	L415	K416	L417	Y418	L419	K420	L421	Y422	L423	K424	L425	Y426	L427	K428	L429	Y430	L431	K432	L433	Y434	L435	K436	L437	Y438	L439	K440	L441	Y442	L443	K444	L445	Y446	L447	K448	L449	Y450	L451	K452	L453	Y454	L455	K456	L457	Y458	L459	K460	L461	Y462	L463	K464	L465	Y466	L467	K468	L469	Y470	L471	K472	L473	Y474	L475	K476	L477	Y478	L479	K480	L481	Y482	L483	K484	L485	Y486	L487	K488	L489	Y490	L491	K492	L493	Y494	L495	K496	L497	Y498	L499	K500	L501	Y502	L503	K504	L505	Y506	L507	K508	L509	Y510	L511	K512	L513	Y514	L515	K516	L517	Y518	L519	K520	L521	Y522	L523	K524	L525	Y526	L527	K528	L
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Chain E:

I313	I223	Y131	V2
	D230	E132	V3
H316		E133	
	V239	D134	K8
		L135	P9
	N244	E136	R16
	R245	K137	
	F246		R23
		E142	K24
	F249		K24
		Q148	G28
	L253	R149	I29
	H254	L150	
		M154	K34
	N257	L155	
	K258	Q156	S44
	G259		
	L260	K160	L88
	G261		F59
	T262	E163	
		M166	H62
	K265		L63
	T266		
	L267	D173	L71
	L271	A174	
		A175	E76
	R274	A176	A77
		I177	
	D278	Y178	L80
	L279	Q179	A81
	A280	A180	L82
	N281		L83
	T282	Q184	R84
	K283	I185	K85
	E284	G186	
	F285	T187	F89
	T286	D188	
	Q287	E189	H95
	A288	S190	
		V195	L101
	G291		G102
	K292	T198	K105
	S293	R199	N106
	L294	S200	A107
	F297	Q203	T111
	T298	L204	
	A299		S116
	D300	F208	N117
	D301		A118
	C302	S215	Q119
		K216	T120
	K307	K217	H121
	D308	T218	
	L310	T219	K124
	L311	L220	
	C312	Q221	L129
		A222	L129

Chain F:

D230	K132	V2
D301	E133	V3
G302	D134	Q4
K307	L135	F13
D308	E136	N14
L309	E138	S15
I313	I139	R16
H316	L140	E17
	S141	L22
	F147	R23
	L150	K24
	M154	I29
	K160	T37
	E161	R43
	E163	R48
	M166	F59
D278	I177	L63
L279	E182	K68
N281	G183	E76
I282	L184	A77
K283	G186	L80
E284	T187	A81
T285	D188	L82
M289	E189	K85
F297	F192	P86
D300	V195	D87
D301	L196	E88
G302	A197	N98
K307	T198	K99
D308	R199	G100
L309	S200	L101
I313	Q203	G102
H316	L204	K105
	H205	D110
	H209	T114
	K213	Q115
	N216	T120
	K217	H121
	L220	A122
	N225	K128
	E226	E131

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.94Å 162.54Å 188.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.93	Depositor
% Data completeness (in resolution range)	92.5 (10.00-1.93)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.208 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15709	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2498	0.79	0/3360
1	B	0.32	0/2498	0.85	1/3360 (0.0%)
1	C	0.32	0/2498	0.87	6/3360 (0.2%)
1	D	0.32	0/2498	0.88	4/3360 (0.1%)
1	E	0.30	0/2498	0.88	9/3360 (0.3%)
1	F	0.32	0/2498	0.84	5/3360 (0.1%)
All	All	0.32	0/14988	0.85	25/20160 (0.1%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	E	199	ARG	CD-NE-CZ	12.15	140.61	123.60
1	E	199	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	D	199	ARG	CD-NE-CZ	9.71	137.19	123.60
1	F	199	ARG	NE-CZ-NH1	9.68	125.14	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2462	0	2457	71	0
1	B	2462	0	2457	64	0
1	C	2462	0	2457	50	0
1	D	2462	0	2457	69	0
1	E	2462	0	2457	75	0
1	F	2462	0	2457	65	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	140	0	0	7	0
3	B	193	0	0	5	0
3	C	173	0	0	6	0
3	D	152	0	0	3	0
3	E	117	0	0	9	0
3	F	151	0	0	6	0
All	All	15709	0	14742	364	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 364 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:260:LEU:CD1	1:D:260:LEU:HD13	1.45	1.44
1:B:260:LEU:HD12	1:D:260:LEU:CD1	1.59	1.30
1:B:260:LEU:CD1	1:D:260:LEU:CD1	2.19	1.10
1:F:82:LEU:HD11	1:F:313:ILE:HD11	1.39	1.01
1:E:82:LEU:HD11	1:E:313:ILE:HD11	1.44	1.00

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 X-ray entries followed by that with respect to entries of similar resolution. 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	313/315 (99%)	302 (96%)	10 (3%)	1 (0%)	50	37
1	B	313/315 (99%)	303 (97%)	7 (2%)	3 (1%)	22	9
1	C	313/315 (99%)	305 (97%)	8 (3%)	0	100	100
1	D	313/315 (99%)	305 (97%)	8 (3%)	0	100	100
1	E	313/315 (99%)	305 (97%)	8 (3%)	0	100	100
1	F	313/315 (99%)	304 (97%)	8 (3%)	1 (0%)	50	37
All	All	1878/1890 (99%)	1824 (97%)	49 (3%)	5 (0%)	50	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLY
1	B	258	LYS
1	B	259	GLY
1	B	262	THR
1	F	101	LEU

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 X-ray entries followed by that with respect to entries of similar resolution. 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	260/260 (100%)	238 (92%)	22 (8%)	15	4
1	B	260/260 (100%)	241 (93%)	19 (7%)	20	6
1	C	260/260 (100%)	238 (92%)	22 (8%)	15	4
1	D	260/260 (100%)	235 (90%)	25 (10%)	12	2
1	E	260/260 (100%)	232 (89%)	28 (11%)	9	2
1	F	260/260 (100%)	233 (90%)	27 (10%)	10	2
All	All	1560/1560 (100%)	1417 (91%)	143 (9%)	13	3

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	ARG
1	D	216	ASN

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Mol	Chain	Res	Type
1	F	217	LYS
1	D	29	ILE
1	D	132	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	10	HIS
1	D	203	GLN
1	F	203	GLN
1	D	62	HIS
1	D	205	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.