



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 7, 2017 – 03:04 AM EDT

PDB ID : 5WEM
EMDB ID: : EMD-8821
Title : GluA2 bound to GSG1L in digitonin, state 1
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on : unknown
Resolution : 6.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

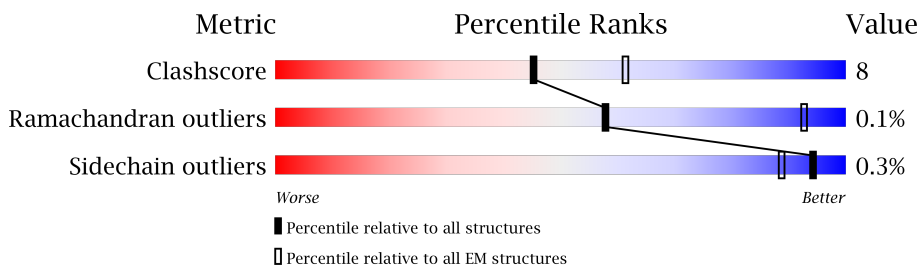
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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
Sidechain outliers	121581	1026

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	1057	71% 19% 9%
1	B	1057	57% 17% 26%
1	C	1057	71% 19% 9%
1	D	1057	58% 16% 26%

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 27360 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 Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	962	7555	4864	1248	1401	42	0	0
1	B	780	6125	3932	1011	1152	30	0	0
1	C	962	7555	4864	1248	1401	42	0	0
1	D	780	6125	3932	1011	1152	30	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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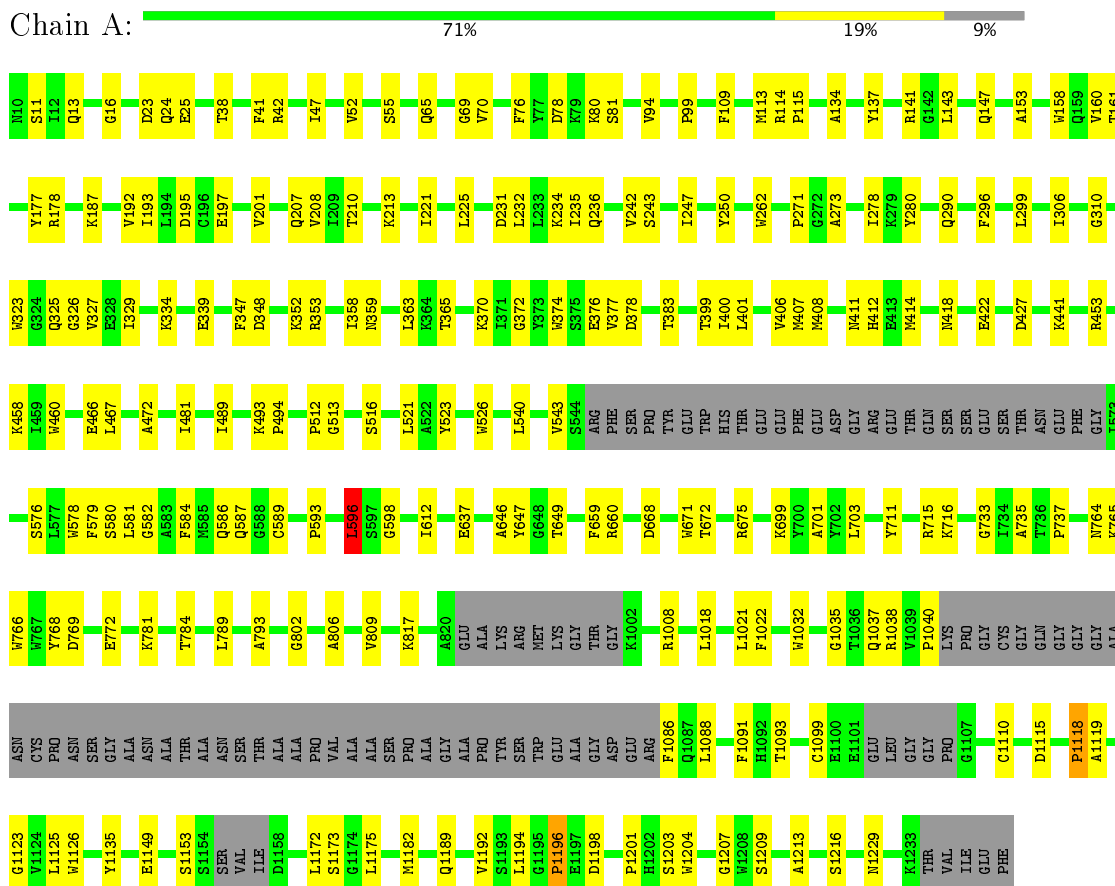
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
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C	384	GLU	GLY	engineered mutation	UNP P19491
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C	392	GLN	ASN	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	1151	LEU	VAL	engineered mutation	UNP D3Z7H4

3 Residue-property plots

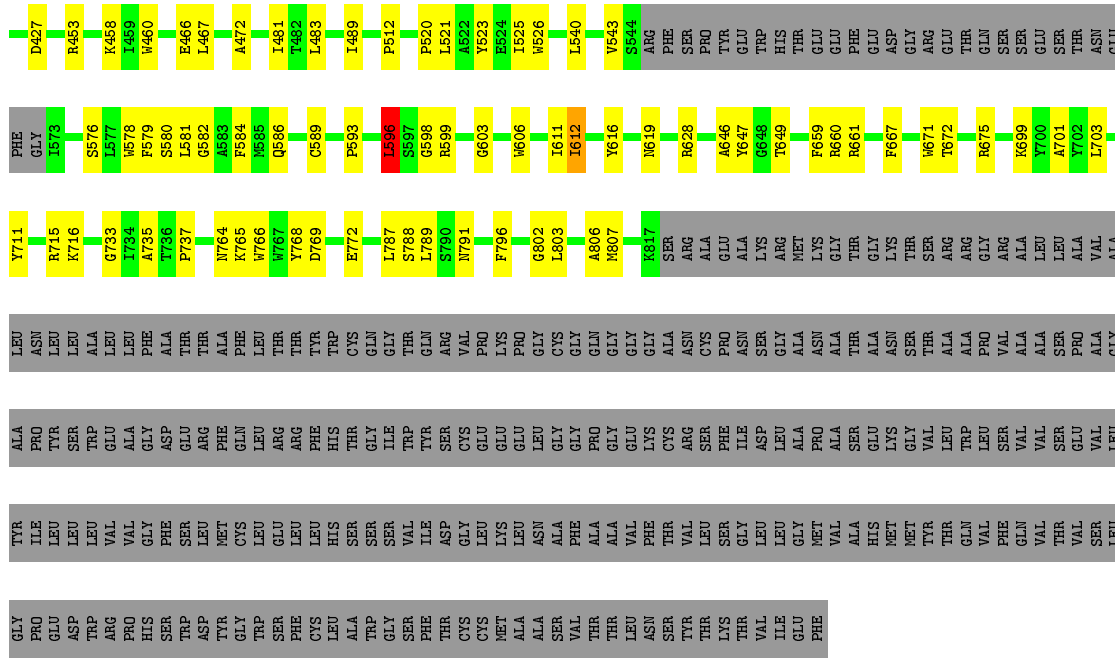
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein

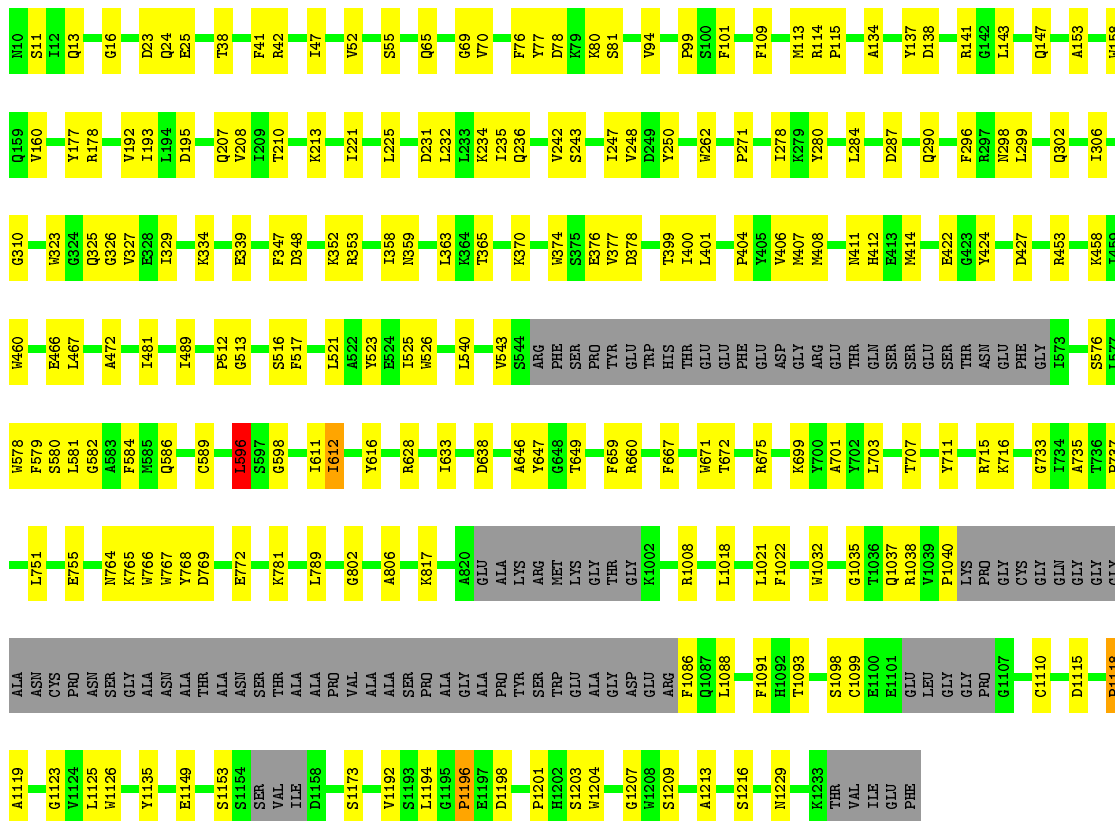


- Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein





- Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein



- Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein



H10	S11	I12	Q13	G16	D23	Q24	E25	T38	F41	R42	I47	V52	S55	Q65	G69	V70	F76	Y77	D78	K79	K80	V94	P99	S100	F101	F109	M113	R114	P115	A134	Y137	R141	G142	L143	Q147	A153	W158	Q159	V160												
T161	Y177	R178	K187	V192	I193	L194	D195	G196	E197	V201	Q207	V208	L209	T210	K213	I221	L225	D231	L232	L233	K234	L235	Q236	V242	S243	L247	Y250	V262	V262	HIS	V377	D378	T383	T399	I400	L401	V406	M407	M408	L284	D287	M411	H412	E413	M414	F296					
R297	M298	L299	Q302	I306	G310	W323	G324	Q325	G326	V327	I329	K334	E339	F347	D348	K352	R353	I358	N359	L363	K364	T365	K370	I371	G372	T373	W374	S375	E376	V377	D378	T383	T399	I400	L401	V406	M407	M408	L284	D287	M411	H412	E413	M414	F296						
E422	R453	K458	L459	W460	E466	L467	K471	A472	I481	I489	K493	P512	F517	P520	L521	A522	Y523	W526	L540	V543	ARG	PHE	SER	PRO	TYR	TRP	HIS	V377	D378	T383	T399	I400	L401	V406	M407	M408	L284	D287	M411	H412	E413	M414	F296								
GLU	PHE	GLY	I573	S576	W578	F579	S580	L581	G582	A583	F584	G588	C589	P593	E596	S597	G598	V601	M619	R628	Y647	G648	T649	F659	R660	F667	D668	W671	T672	R675	A701	Y702	L703	Y711	R715	K716	G733	I734	A735	T736	P737										
W764	K765	Y768	D769	E772	K776	L787	S788	L789	S790	W791	G802	A806	R817	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS	THR	GLY	LYS	THR	ARG	ARG	GLY	PRO	VAL	ALA	LEU	LEU	ALA	VAL	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU					
THR	THR	TYR	TRP	CYS	GLN	GLY	THR	GLN	ARG	VAL	VAL	PRO	LYS	PRO	GLY	GLY	CYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
ARG	ARG	PHE	HIS	THR	THR	GLY	ILE	TRP	THR	TYR	THR	ASP	CYS	VAL	GLY	GLY	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO
GLU	LEU	HIS	SER	SER	VAL	ILE	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
SER	PHE	CYS	LEU	ALA	THR	GLY	SER	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	20392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.30	1/7718 (0.0%)	0.50	1/10438 (0.0%)
1	B	0.29	0/6253	0.50	1/8450 (0.0%)
1	C	0.30	1/7718 (0.0%)	0.50	1/10438 (0.0%)
1	D	0.30	0/6253	0.50	2/8450 (0.0%)
All	All	0.30	2/27942 (0.0%)	0.50	5/37776 (0.0%)

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	A	0	8
1	B	0	4
1	C	0	7
1	D	0	3
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	612	ILE	C-N	6.91	1.50	1.34
1	A	612	ILE	C-N	-6.54	1.19	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	LEU	CA-CB-CG	8.06	133.84	115.30
1	A	596	LEU	CA-CB-CG	8.03	133.78	115.30
1	D	596	LEU	CA-CB-CG	8.03	133.77	115.30
1	B	596	LEU	CA-CB-CG	8.02	133.74	115.30
1	D	512	PRO	C-N-CA	-5.72	110.30	122.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1118	PRO	Peptide
1	A	378	ASP	Peptide
1	A	593	PRO	Peptide
1	A	781	LYS	Peptide
1	A	817	LYS	Mainchain

5.2 Too-close contacts [i](#)

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	7555	0	7535	120	0
1	B	6125	0	6110	110	0
1	C	7555	0	7536	126	0
1	D	6125	0	6110	98	0
All	All	27360	0	27291	423	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 8.

The worst 5 of 423 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)
1:B:606:TRP:HZ2	1:C:586:GLN:H	1.27	0.78
1:D:596:LEU:HD22	1:D:598:GLY:H	1.55	0.71
1:C:596:LEU:HD22	1:C:598:GLY:H	1.55	0.71
1:A:596:LEU:HD22	1:A:598:GLY:H	1.55	0.70
1:B:596:LEU:HD22	1:B:598:GLY:H	1.55	0.70

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	950/1057 (90%)	888 (94%)	60 (6%)	2 (0%)	51	84
1	B	776/1057 (73%)	728 (94%)	48 (6%)	0	100	100
1	C	950/1057 (90%)	886 (93%)	62 (6%)	2 (0%)	51	84
1	D	776/1057 (73%)	729 (94%)	47 (6%)	0	100	100
All	All	3452/4228 (82%)	3231 (94%)	217 (6%)	4 (0%)	58	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1204	TRP
1	C	1204	TRP
1	A	1119	ALA
1	C	1119	ALA

5.3.2 Protein sidechains [i](#)

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	816/888 (92%)	814 (100%)	2 (0%)	94	97
1	B	662/888 (74%)	660 (100%)	2 (0%)	94	96
1	C	816/888 (92%)	814 (100%)	2 (0%)	94	97
1	D	662/888 (74%)	660 (100%)	2 (0%)	94	96
All	All	2956/3552 (83%)	2948 (100%)	8 (0%)	94	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	660	ARG
1	D	660	ARG
1	C	660	ARG
1	B	596	LEU
1	C	596	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	GLN
1	C	147	GLN
1	D	83	ASN
1	C	24	GLN
1	D	147	GLN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	612:ILE	C	613:ILE	N	1.19